IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In the matter of an application for a German Patent

with the file reference 103 50 722.1
filed on 30 October 2003
in the name of Covion Organic Semiconductors GmbH, Frankfurt, Germany,

and in the matter of an application for a United States Patent.

I, Dr. Ashwood Stephen DRANE, B.Sc., Ph.D., BDÜ, translator to SD Translations Ltd. of Beechwood, Chivery, Tring, Hertfordshire, HP23 6LD, England, do solemnly and sincerely declare:

1. That I am a citizen of the United Kingdom of Great Britain and Northern Ireland.

2. That I am well acquainted with the German and English languages and am a competent translator thereof.

3. That the following is to the best of my knowledge and belief a true and correct translation of the above-referenced patent application and the Official Certificate attached thereto

Dated this 31st day of July 2009

Dr. Ashwood Stephen Drane

FEDERAL REPUBLIC OF GERMANY

Priority certificate regarding the filing of a patent application

File reference: 103 50 722.1

Date of filing: 30 October 2003

Applicant/proprietor: Covion Organic Semiconductors GmbH, 65929 Frankfurt/DE

Title: Metal complexes

IPC: C 07 F, H 01 L

The attached pages are a correct and accurate reproduction of the original documents of this patent application.

Seal

Munich, 6 December 2004
German Patent and Trademark Office
On behalf of
The President

[signature]

Agurks

COVION Organic Semiconductors GmbH C03034

Description

Metal complexes

Chelate complexes and organometallic compounds will be used in the near future as active components (functional materials) as functional components in a number of applications of different types which can be ascribed to the electronics industry in the broadest sense.

In the case of organic electroluminescent devices based on organic components (general description of the construction cf. US-A-4,539,507 and US-A-5,151,629), and individual components thereof, the organic light-emitting diodes (OLEDs), the market introduction has already taken place, as confirmed by the car radios and digital cameras with an "organic display" from the Pioneer and Kodak companies. Further products of this type are just about to be introduced. In spite of everything, significant improvements are still necessary here in order to make these displays a true competitor to or to surpass the liquid-crystal displays (LCDs) which currently dominate the market.

A development in this respect is the improvement of electron-transport materials and blue singlet emitters based on metal chelate complexes, with aluminium and lanthanum chelate complexes being of particular interest here.

A further development that has emerged in recent years is the use of organometallic complexes which exhibit phosphorescence instead of fluorescence [M. A. Baldo, S. Lamansky, P. E. Burrows, M. E. Thompson, S. R. Forrest, Applied Physics Letters, **1999**, *75*, 4-6].

For theoretical spin-statistical reasons, an up to four-fold energy and power efficiency is possible using organometallic compounds as phosphorescence emitters. Whether this new development will succeed is highly dependent on whether it is possible to find corresponding device compositions which are also able to implement these advantages (triplet emission = phosphorescence compared with singlet emission = fluorescence) in the OLEDs. Essential conditions for practical application which may be mentioned here are, in particular, a long operating lifetime, high stability to heating and a low use and operating voltage in order to enable mobile applications.

In both cases, efficient chemical access to the corresponding chelate complexes or organometallic compounds must be possible. However, this is of particular interest

against the background of scarcity of the noble metals ruthenium, osmium, rhodium, iridium, palladium, platinum, and gold.

To date, two basic types of construction of OLEDs, which comprise fluorescence or phosphorescence emitters as colouring components, which differ in their layer structure, have been described in the literature. These OLED types are described in detail, for example, in DE 10261545.4.

The characteristic data of the OLEDs in accordance with the prior art exhibit, inter alia, the following weak points:

1. The operating lifetime is in most cases still much too short, which stands in the way of a market introduction of OLEDs.
2. It is evident from the efficiency/luminance curves that the efficiency frequently drops considerably with increasing luminance. This means that the great luminances that are necessary in practice can only be achieved by high power consumption. However, large power consumptions require high battery powers of portable equipment (mobile phones, laptops, etc.). In addition, the large power consumption, which is for the most part converted into heat, may result in thermal damage to the display.

In the OLED device explained above, the above-mentioned functional materials have been or are being intensively optimised.

For some time, metal complexes have been employed as ETL (for example AlQ_3, C. W. Tang et al., Applied Phys. Lett., **1987**, *51*(12), 913; ZnQ_2 S.-J. Jung et al., J. Korean Electrochemical Society **2000**, *3*(1), 1), HBL (for example B-AlQ_3, R. Kwong et al., Applied Physics Letters, **2002**, *81*(1), 162), as matrix material in the EL (for example B-AlQ_3, C. H. Chen et. al., Proceedings of SPIE-The International Society for Optical Engineering, **1998**, *3421*, 78), as singlet emitter (for example AlQ_3, ZnQ_2 and other complexes, S. Tokito et al., Synthetic Metals, **2000**, *111 - 112*, 393) and as triplet emitter (for example $Ir(PPy)_3$, WO 00/70655; for example $Ir(TPy)_3$ and $Ir(BTPy)_3$, S. Okada et al., Proceedings of the SID, **2002**, *52.2*, 1360). Triplet emitters based on platinum complexes have likewise been known for some time, whwere, besides those of bidentate ligands (for example Brooks et al. Inorg. Chem., **2002**, *41*, 3055-3066), those of tetradentate macrocyclic ligands (for example PtOEP, L. R. Milgrom Polyhedron, **1988**, *7*(1), 57; M. A. Baldo, Nature (London), **1998**, *395*(6698), 151-154) are also known. These complexes of divalent platinum (d^8 configuration) cited above have, like the majority of platinum(II) complexes, a

planar or virtually planar structure. In solids, these planar complex units aggregate in such a way that strong and frequently cooperative ligand-ligand, metal-metal or ligand-metal interactions occur.

Besides the individual weak points that are specific to each molecule, the class of the known metal complexes has general weak points, which are described briefly below.

1. Many of the known metal complexes, in particular those which contain main-group metals, such as aluminium, or transition metals having the d^{10} configuration, such as zinc, have a sometimes considerable hydrolysis sensitivity, which can be so pronounced that the metal complex is significantly decomposed even after brief exposure to air.
   Others, by contrast, such as, for example, the AlQ_3 and ZnQ_2 used as electron-transport material, tend to adduct water.
   The high hygroscopicity of these and similar aluminium and zinc complexes is a crucial practical disadvantage. AlQ_3 which is synthesised and stored under normal conditions, always also contains one molecule of water per complex molecule in addition to the hydroxyquinoline ligands [cf., for example: H. Schmidbaur et al., Z. Naturforsch., **1991**, *46b*, 901-911]. This water is extremely difficult to remove. For use in OLEDs, AlQ_3 and ZnQ_2 therefore have to be subjected to complex purification in complicated, multistep sublimation processes and subsequently stored and handled under a protective-gas atmosphere with exclusion of water. Furthermore, large variations in the quality of individual AlQ_3 batches and poor storage stability have been observed (see: S. Karg, E-MRS Conference, 2000, Strasburg).
2. Many of the known metal complexes have low thermal stability. During vacuum deposition of the metal complexes, this inevitably always results in the liberation of organic pyrolysis products, which in some cases, even in small amounts, considerably shorten the operating lifetime of the OLEDs (see, for example, R.G.Charles, J. Inorg. Nucl. Chem., **1963**, *25*, 45; via the thermal stability of MQ_2, where M is a divalent metal, such as, for example, Zn).
3. The strong interaction of the complex units in solids, for example in the case of planar complexes of d^8 metals, such as platinum(II), likewise causes aggregation of the complex units in the emitter layer if the degree of doping exceeds about 0.1%, which is the case in accordance with the current state of the art. This aggregation results in the formation of so-called excimers or exciplexes on excitation (optical or electric). These aggregates frequently have an unstructured, broad emission band, which makes the production of the purest possible primary

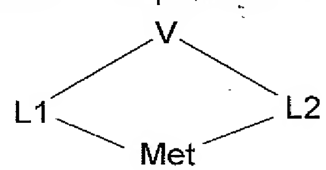
colours (RGB) considerably more difficult or completely impossible. In general, the efficiency for this transition also drops.

4. In addition, it is evident from the above that the emission colour is highly dependent on the degree of doping, a parameter which can only be controlled to a certain extent with considerable technical effort, in particular in large production plants.

There was therefore a demand for alternative compounds which do not have the above-mentioned weak points.

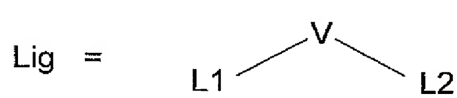
This class of metal complexes described below and the use thereof as functional materials in electro-optical components is novel and has not been described in the literature to date, but their efficient preparation and availability as pure substance is of great importance for this.

The present invention thus relates to compounds of structure 1



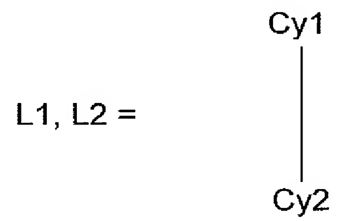
structure 1

characterised in that they contain a metal Met, coordinated to a tetradentate ligand Lig of structure 2



structure 2

where V is a bridging unit, characterised in that it contains 1 to 40 atoms heavier than hydrogen and connects the two ligand moieties L1 and L2, which may be identical or different on each occurrence, covalently to one another, and where the two ligand moieties L1 and L2, satisfy structure 3



structure 3

where Cy1 and Cy2, identically or differently on each occurrence, each correspond to a substituted or unsubstituted, saturated, unsaturated or aromatic homo- or heterocycle, preferably an aromatic ring, which is in each case bonded ionically, covalently or coordinatively to the metal (Met) via a ring atom or via an atom bonded exocyclically to the homo- or heterocycle.

The bridge V is characterised in that it promotes the formation of monocyclic metal complexes of structure 1 or the formation of coordination polymers does not occur or only occurs to a minor extent on reaction of the ligand of structure 2 with metal compounds.

The homo- or heterocycles Cy1 and Cy2 may be linked to one another via substituents and thus form a polycyclic, aliphatic or aromatic ring system.

Preference is given to compounds of structure 1 according to the invention which are characterised in that they are electrically neutral.

Preference is given to compounds of structure 1 according to the invention which are characterised in that L1 = L2.

Preference is given to compounds of structure 1 according to the invention, characterised in that the linking unit V contains one, two or three bridging atoms or is a 3- to 6-membered homo- or heterocycle.

Preference is given to compounds of structure 1 according to the invention, characterised in that the linking unit V contains a linking atom selected from the 3rd, 4th, 5th or 6th main group.

Particular preference is given to linking units V in which V stands for BR^1, $-(CR_2)R^1B(CR_2)-$, $-(CR_2CR_2)R^1B(CR_2CR_2)-$, C=O, $C{=}NR^1$, C=S, CR_2, CR(OH), $CR(OR^1)$, $C(NR^1)_2$, $-(CR_2)R_2C(CR_2)-$, $-(CR_2CR_2)R_2C(CR_2CR_2)-$, $-(SiR_2)R_2C(SiR_2)-$, $-(SiR_2CR_2)R_2C(SiR_2CR_2)-$, $-(CR_2SiR_2)R_2C(CR_2SiR_2)-$, $-(SiR_2SiR_2)R_2C(SiR_2SiR_2)-$, cis-

RC=CR, 1,2-C_6H_4, 1,3-C_6H_4, SiR_2, $Si(OH)_2$, $Si(OR^1)_2$, -$(CR_2)R_2Si(CR_2)$-, -$(CR_2CR_2)R_2Si(CR_2CR_2)$-, -$(SiR_2)R_2Si(SiR_2)$-, -$(SiR_2CR_2)R_2Si(SiR_2CR_2)$-, -$(CR_2SiR_2)R_2Si(CR_2SiR_2)$-, -$(SiR_2SiR_2)R_2Si(SiR_2SiR_2)$-, R^1N, -$(CR_2)R^1N(CR_2)$-, -$(CR_2CR_2)R^1N(CR_2CR_2)$-, FP, FPO, R^1P, R^1As, R^1Sb, R^1Bi, R^1PO, R^1AsO, R^1SbO, R^1BiO, R^1PSe, R^1AsSe, R^1SbSe, R^1BiSe, R^1PTe, R^1AsTe, R^1SbTe, R^1BiTe, O, S, Se, -$(CR_2)O(CR_2)$-, -$(CR_2)S(CR_2)$-, -$(CR_2)(O)S(CR_2)$-, -$(CR_2)(O)_2S(CR_2)$-;

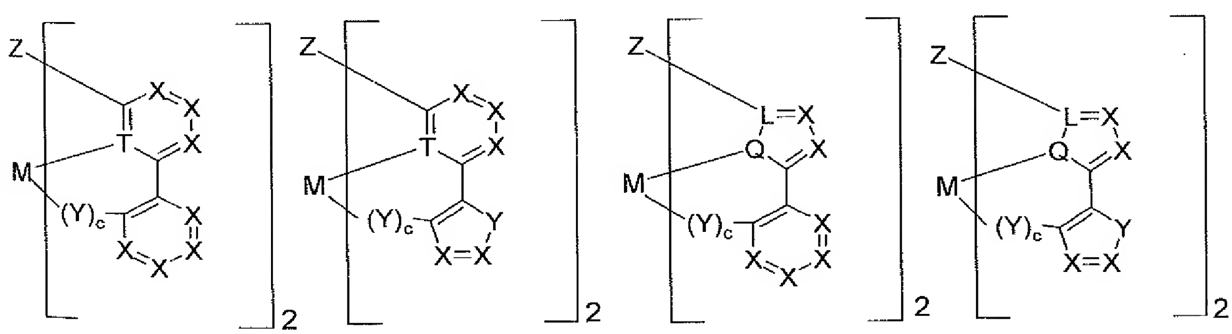
and

R is, identically or differently on each occurrence, H, F, Cl, Br, I, NO_2, CN, a straight-chain, branched or cyclic alkyl or alkoxy group having 1 to 20 C atoms, where one or more non-adjacent CH_2 groups may be replaced by -O-, -S-, -NR^1- or –$CONR^2$- and where one or more H atoms may be replaced by F, or an aryl or heteroaryl group having 1 to 14 C atoms, which may be substituted by one or more non-aromatic radicals R, where a plurality of substituents R, both on the same ring and also on the two different rings, may in turn form a further mono- or polycyclic, aliphatic or aromatic ring system; and

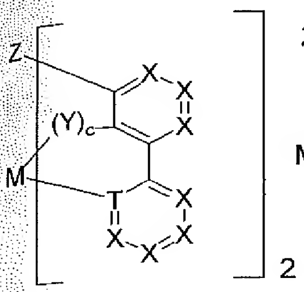
R^1 and R^2, identically or differently on each occurrence, denote H or an aliphatic or aromatic hydrocarbon radical having 1 to 20 C atoms.

Particular preference is given to metal complexes as per compounds (1) to (8) according to Scheme 1,

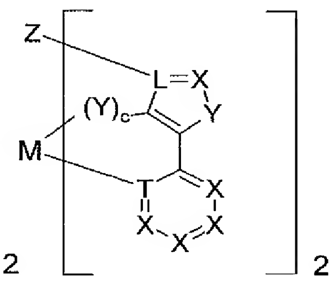
Scheme 1:



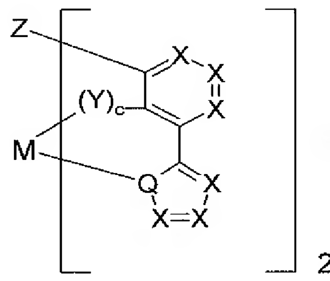
compounds (1) **compounds (2)** **compounds (3)** **compounds (4)**



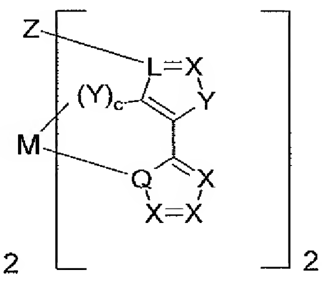
compounds (5)



compounds (6)



compounds (7)



compounds (8)

where the symbols and indices have the following meaning:

M Be, Mg, Ca, Sr, Ba, Cr, Mo, W, Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag, Au, Zn, Cd, Hg;

L is, identically or differently on each occurrence, C, N, P;

Q is, identically or differently on each occurrence, N, O, S, Se, Te;

T is, identically or differently on each occurrence, N, P;

X is, identically or differently on each occurrence, CR, N, P;

Y is, identically or differently on each occurrence, NR^1, O, S, Se, Te, SO, SeO, TeO, SO_2, SeO_2, TeO_2;

Z BR^1, $-(CR_2)R^1B(CR_2)-$, $-(CR_2CR_2)R^1B(CR_2CR_2)-$, C=O, $C=NR^1$, C=S, CR_2, CR(OH), $CR(OR^1)$, $C(NR^1)_2$, $-(CR_2)R_2C(CR_2)-$, $-(CR_2CR_2)R_2C(CR_2CR_2)-$, $-(SiR_2)R_2C(SiR_2)-$, $-(SiR_2CR_2)R_2C(SiR_2CR_2)-$, $-(CR_2SiR_2)R_2C(CR_2SiR_2)-$, $-(SiR_2SiR_2)R_2C(SiR_2SiR_2)-$, cis-RC=CR, 1,2-$C_6H_4$, 1,3-$C_6H_4$, SiR_2, $Si(OH)_2$, $Si(OR^1)_2$, $-(CR_2)R_2Si(CR_2)-$, $-(CR_2CR_2)R_2Si(CR_2CR_2)-$, $-(SiR_2)R_2Si(SiR_2)-$, $-(SiR_2CR_2)R_2Si(CR_2SiR_2)-$, $-(CR_2SiR_2)R_2Si(SiR_2CR_2)-$, $-(SiR_2SiR_2)R_2Si(SiR_2SiR_2)-$, R^1N, $-(CR_2)R^1N(CR_2)-$, $-(CR_2CR_2)R^1N(CR_2CR_2)-$, FP, FPO, R^1P, R^1As, R^1Sb, R^1Bi, R^1PO, R^1AsO, R^1SbO, R^1BiO, R^1PSe, R^1AsSe, R^1SbSe, R^1BiSe, R^1PTe, R^1AsTe, R^1SbTe, R^1BiTe, O, S, Se, $-(CR_2)O(CR_2)-$, $-(CR_2)S(CR_2)-$, $-(CR_2)(O)S(CR_2)-$, $-(CR_2)(O)_2S(CR_2)-$;

R is, identically or differently on each occurrence, H, F, Cl, Br, I, NO_2, CN, a straight-chain, branched or cyclic alkyl or alkoxy group having 1 to 20 C atoms, where one or more non-adjacent CH_2 groups may be replaced by -O-, -S-, $-NR^1-$ or $–CONR^2-$ and where one or more H atoms may be replaced by F, or an aryl or heteroaryl group having 1 to 14 C atoms, which may be substituted by one or more non-aromatic radicals R, where a plurality of substituents R, both on the same ring and also on the two different

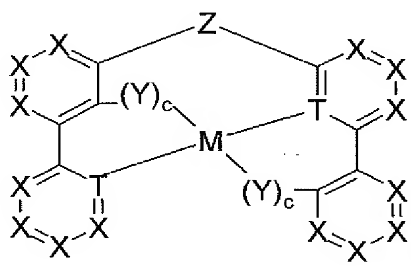
rings, may in turn form a further mono- or polycyclic, aliphatic or aromatic ring system; and

R^1 and R^2, identically or differently on each occurrence, are H or an aliphatic or aromatic hydrocarbon radical having 1 to 20 C atoms.

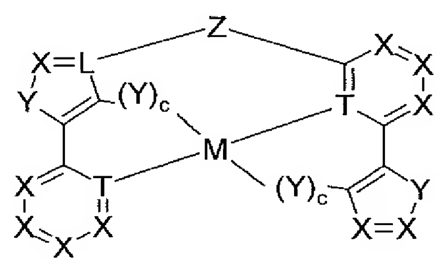
c is, identically or differently on each occurrence, 0 or 1.

In addition, preference is likewise given to compounds (9) to (12) according to Scheme 2,

Scheme 2:



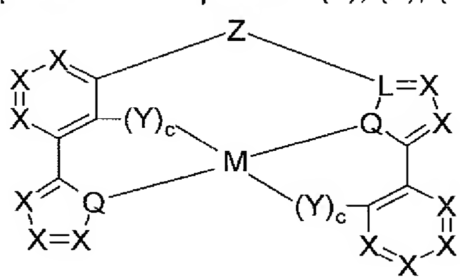
compounds (9)



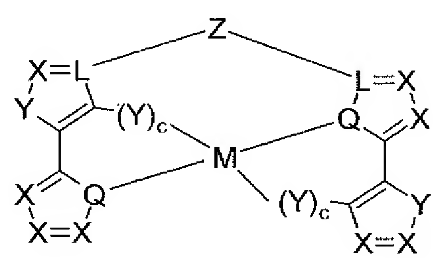
compounds (10)

where the symbols and indices M, L, Q, T, X, Y, Z, R, R^1, R^2 and c have the meaning indicated under Scheme 1.

The invention furthermore relates to compounds which simultaneously have ligands of the type as for compounds (1), (2), (3) and/or (4), i.e. mixed



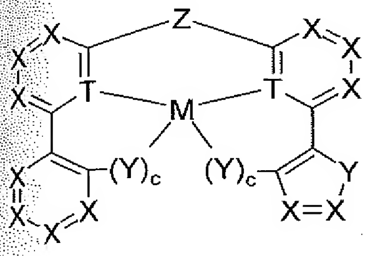
compounds (11)



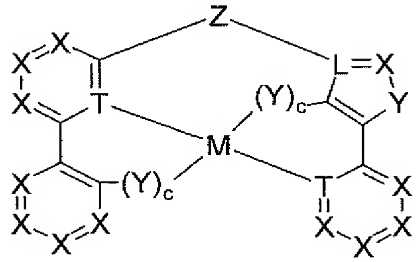
compounds (12)

ligand systems. These are described by the formulae (13) to (30) - according to Scheme 3:

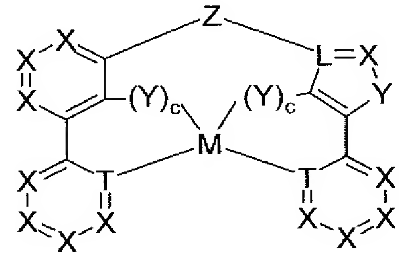
Scheme 3:



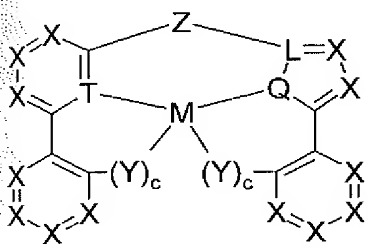
compounds (13)



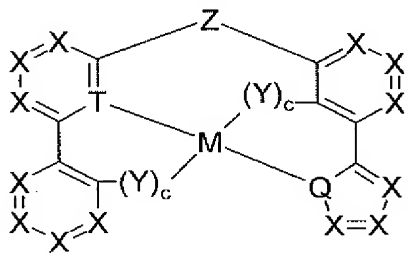
compounds (14)



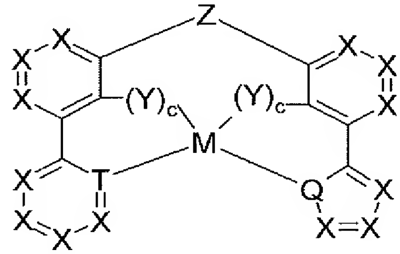
compounds (15)



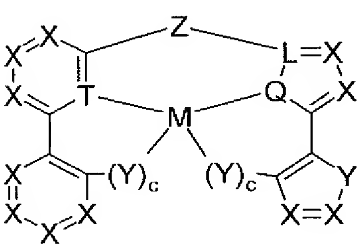
compounds (16)



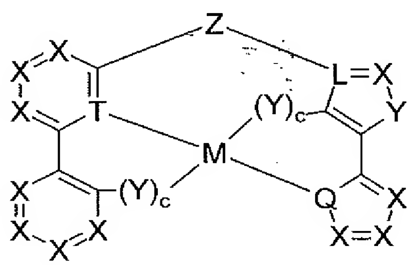
compounds (17)



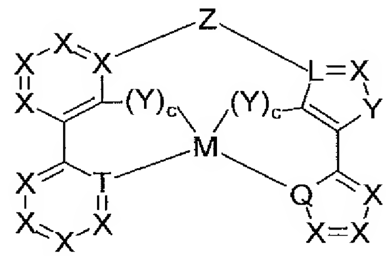
compounds (18)



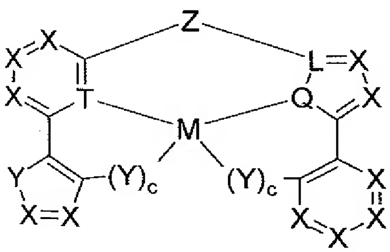
compounds (19)



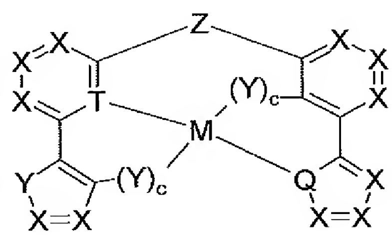
compounds (20)



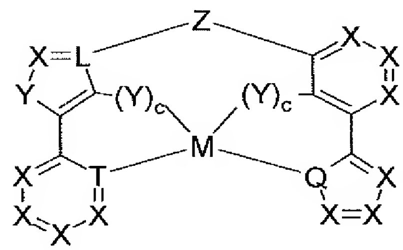
compounds (21)



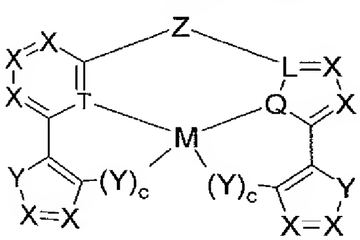
compounds (22)



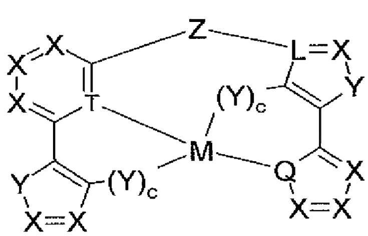
compounds (23)



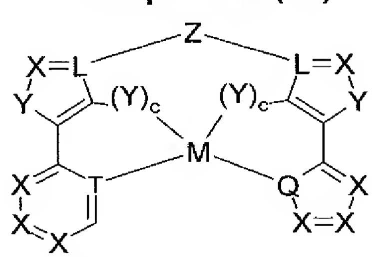
compounds (24)



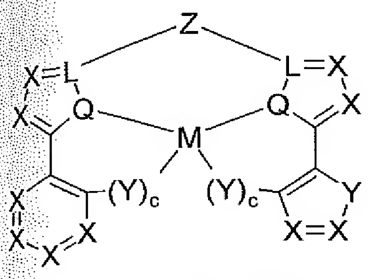
compounds (25)



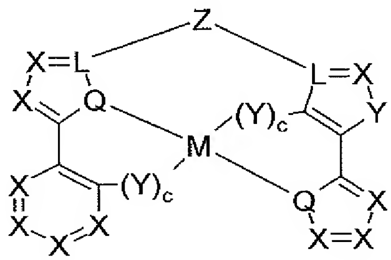
compounds (26)



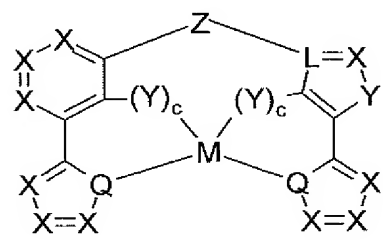
compounds (27)



compounds (28)



compounds (29)



compounds (30)

where the symbols and indices M, L, Q, T, X, Y, Z, R, R^1, R^2 and c have the meaning indicated under Scheme 1.

The compounds of structure 1 or compounds (1) to (30) may optionally carry further mono- or polydentate, cationic, neutral or anionic ligands.

Preference is given to compounds (1) to (30) according to the invention in which the symbol M = Be, Mg, Pt, Zn.

Particular preference is given to compounds (1) to (30) according to the invention in which the number zero stands for c and M = Pt.

Preference is likewise given to compounds (1) to (30) according to the invention in which the symbol L = C, N.

Preference is likewise given to compounds (1) to (30) according to the invention in which the symbol Q = O, S.

Preference is likewise given to compounds (1) to (30) according to the invention in which the symbol T = N.

Preference is likewise given to compounds (1) to (30) according to the invention in which the symbol X = CR, N.

Preference is likewise given to compounds (1) to (30) according to the invention in which the symbol Z = BR^1, CR_2, CO, SiR^1_2, R^1N, FP, FPO, R^1P, R^1PO.
Preference is likewise given to compounds (1) to (30) according to the invention in which R^1 and R^2, identically or differently on each occurrence, denotes H or an aliphatic or aromatic hydrocarbon radical having 1 to 20 C atoms.

Preference is likewise given to compounds (1) to (30) according to the invention in which the symbol R = H, F, Cl, Br, I, CN a straight-chain or branched or cyclic alkyl or alkoxy group having 1 to 6 C atoms or an aryl or heteroaryl group having 3 to 10 C atoms, which may be substituted by one or more non-aromatic radicals R, where a plurality of substituents R, both on the same ring and also on the two different rings, may together in turn form a further mono- or polycyclic, aliphatic or aromatic ring system.

In compounds (1) to (30), the radicals R may form aliphatic, olefinic or aromatic ring systems.

If the radicals R form aromatic ring systems in compounds (1) to (30), these are aromatic preferably benzene, 1- or 2-naphthalene, 1-, 2- or 9-anthracene, 2-, 3- or 4-pyridine, 2-, 4- or 5-pyrimidine, 2-pyrazine, 3- or 4-pyridazine, triazine, 2-, 3-, 4-, 5-, 6-, 7- or 8-quinoline, 2- or 3-pyrrole, 3-, 4-, 5-pyrazole, 2-, 4-, 5-imidazole, 2-, 3-thiophene, 2-, 3-selenophene, 2- or 3-furan, 2-(1,3,4-oxadiazole), indole and carbazole.

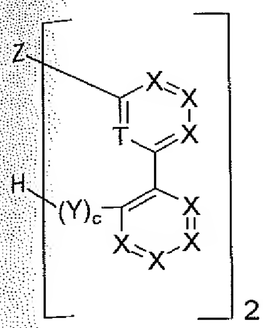
Surprisingly, it has now been found that metal complexes according to the invention with tetradentate chelating, non-macrocyclic ligands exhibit excellent properties on use as ETL, as HBL, as matrix material in the EL, as singlet emitter and also as triplet emitter, where the respective, specific function is determined by the suitable choice of the metal and of the suitable associated ligand. The present invention relates to these compounds. The compounds according to the invention are distinguished by the following general properties:

1. The compounds according to the invention are distinguished - in contrast to many known metal complexes which undergo partial or complete pyrolytic decomposition on sublimation - by high thermal stability. This applies in particular to the platinum complexes according to the invention with tetradentate chelating ligands which, besides dative coordination via a heteroatom, also contain at least one aryl carbon-platinum bond. This high stability of the compounds according to the invention results in a significant increase in the operating lifetime on use in corresponding devices.
2. The compounds according to the invention have no evident hydrolysis or hygroscopicity. Storage for a number of days or weeks with ingress of air and water vapour does not result in any changes to the substances. The adduction of water onto the compounds could not be detected. This has the advantage that the substances can be purified, transported, stored and prepared for use under simpler conditions.

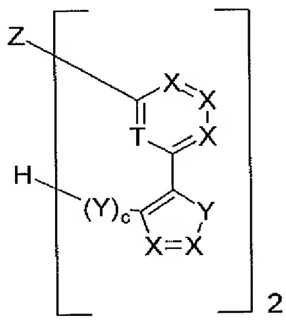
3. The compounds according to the invention - employed as ETL material in electroluminescent devices - result in high efficiencies therein, in particular independently of the current densities used. Very good efficiencies are thus also facilitated even at high current densities.
4. The compounds according to the invention - employed as HBL material in electroluminescent devices - result in high efficiencies therein, in particular independently of the current densities used. Very good efficiencies are thus also facilitated even at high current densities, i.e. high luminances. In addition, the materials according to the invention are stable to holes, which is not the case to an adequate extent, for example, in the case of other metal complexes, for example AlQ_3 and analogous compounds (Z. Popovic et al., Proceedings of SPIE, **1999**, *3797*, 310-315).
5. The compounds according to the invention - employed in electroluminescent devices as EL material in pure form or as EL material doped into a matrix material or as matrix material in combination with a dopant - result in high efficiencies therein, with the electroluminescent devices being distinguished by steep current/voltage curves and particularly by long operating lifetimes.
6. The compounds according to the invention are shaped by the structural definitions in such a way that they are non-planar and thus aggregation with formation of strong metal-metal, metal-ligand or ligand-ligand interactions is suppressed.
7. Suppression of the aggregation of these compounds results firstly in narrow emission bands and thus purer emission colours. Secondly, the emission colour is independent of the degree of doping over broad ranges, which is a major advantage for industrial applications.
8. Without wishing to be tied to a particular theory, the rigid structure of the compounds according to the invention is conducive to high quantum efficiencies of the emission transitions.
9. The compounds according to the invention can be prepared in a readily reproducible manner in reliably high purity and have no batch variations.
10. The compounds according to the invention in some cases have excellent solubility in organic solvents, it being possible for the solubility to be customised through a suitable choice of the substitution pattern, for example by introduction of branched alkyl chains into bridge V or Z. These materials can thus also be processed from solution by coating or printing techniques. Even in the case of conventional processing by evaporation, this property is advantageous since the cleaning of the plants or shadow masks employed by washing is thus considerably simplified.

The present invention likewise relates to compounds (31) to (60), according to Scheme 4:

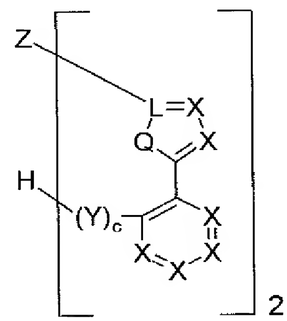
Scheme 4



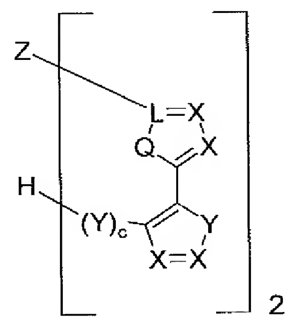
compounds (31)



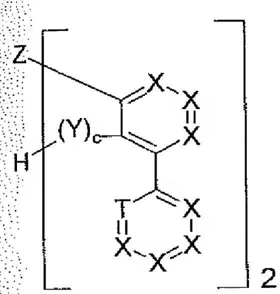
compounds (32)



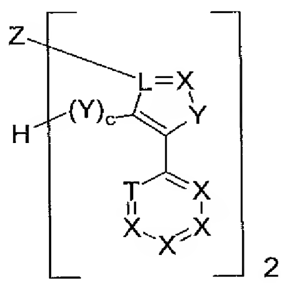
compounds (33)



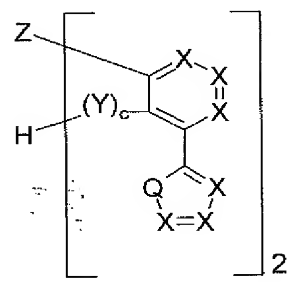
compounds (34)



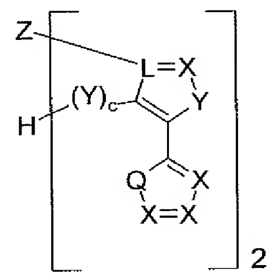
compounds (35)



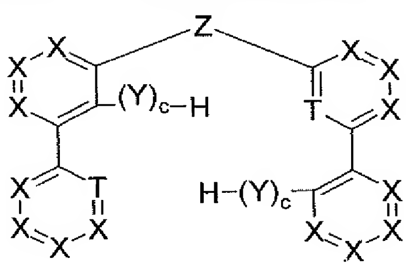
compounds (36)



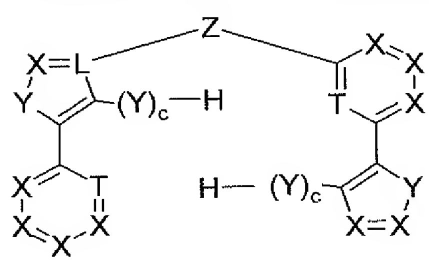
compounds (37)



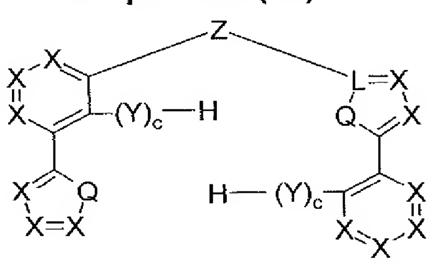
compounds (38)



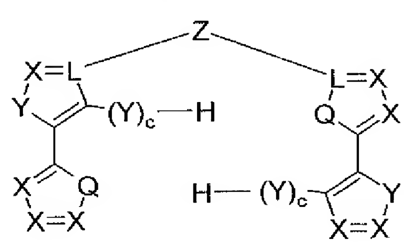
compounds (39)



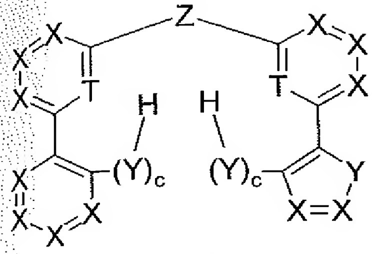
compounds (40)



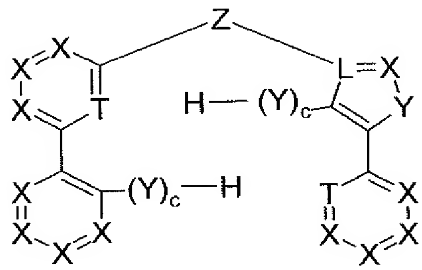
compounds (41)



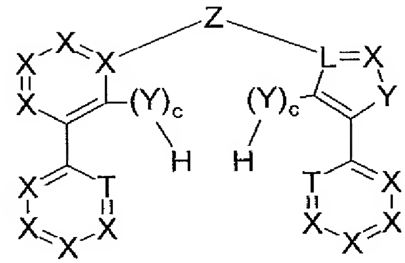
compounds (42)



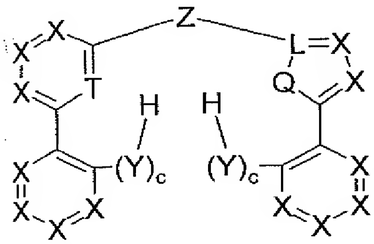
compounds (43)



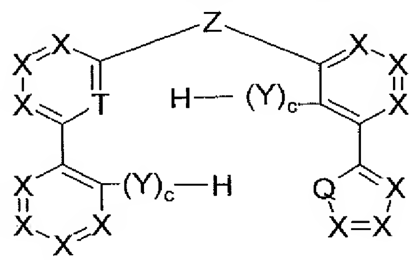
compounds (44)



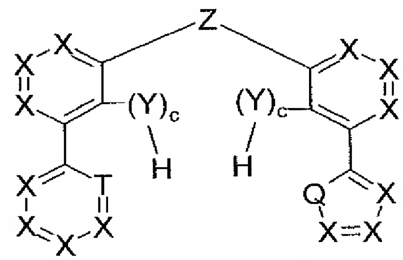
compounds (45)



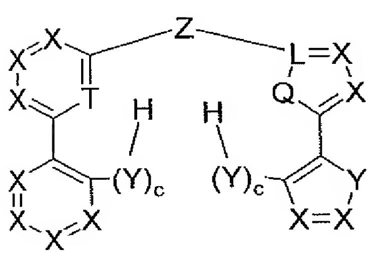
compounds (46)



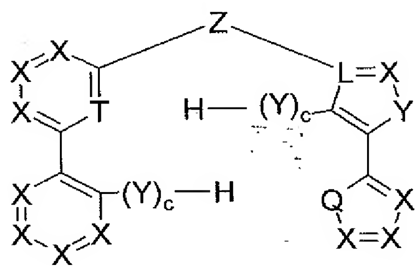
compounds (47)



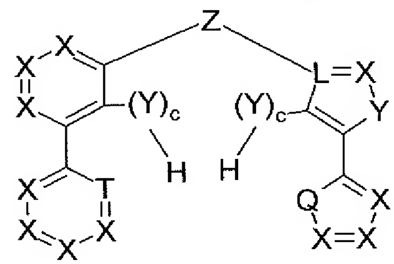
compounds (48)



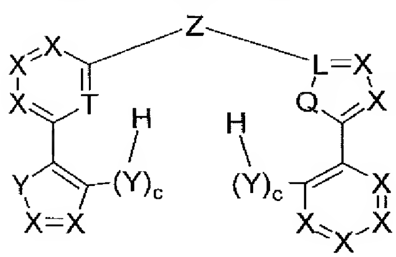
compounds (49)



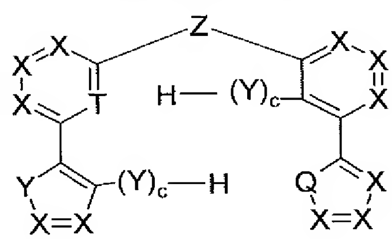
compounds (50)



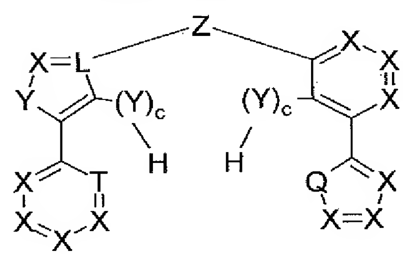
compounds (51)



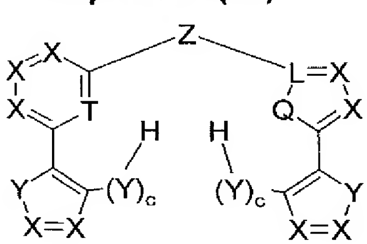
compounds (52)



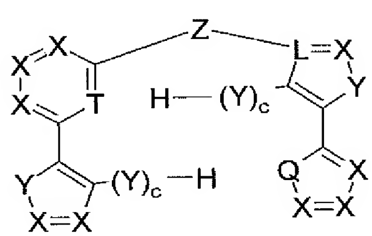
compounds (53)



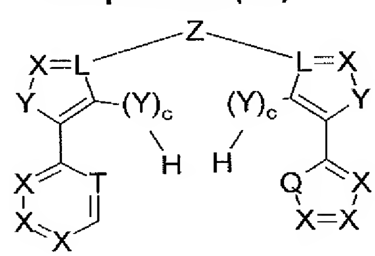
compounds (54)



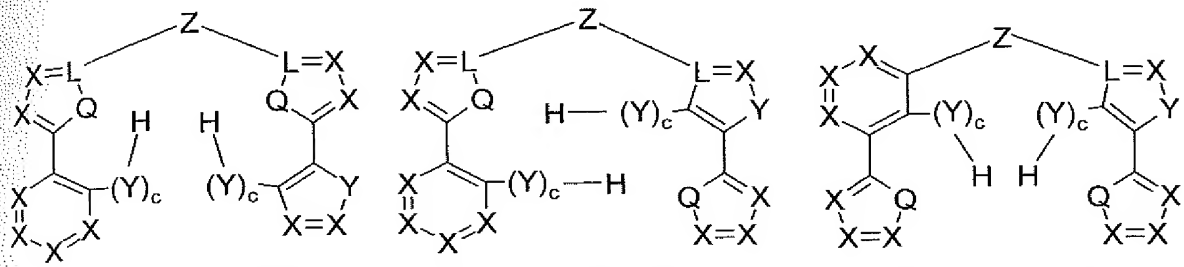
compounds (55)



compounds (56)



compounds (57)



compounds (58) compounds (59) compounds (60)

where the symbols and indices Q, L, T, X, Y, Z, R, R^1, R^2 and c have the meaning indicated under Scheme 1, with the exception of the compounds bis(6-phenyl-2-pyridyl)methane [CAS 362602-93-5], bis(6-phenyl-2-pyridyl) ketone [CAS 217177-35-0], bis(6-(1-hydroxy-3,5-di-tert-butyl)phenyl-2-pyridyl)methanol [CAS 367525-74-4], 2,2′-thiobis(3-cyano-2,4-diphenyl)pyridine [CAS 160598-76-5], bis(6-(3-phenyl)-phenyl-2-pyridyl)methane [CAS 57476-80-9] and isomers [CAS 57476-79-6]

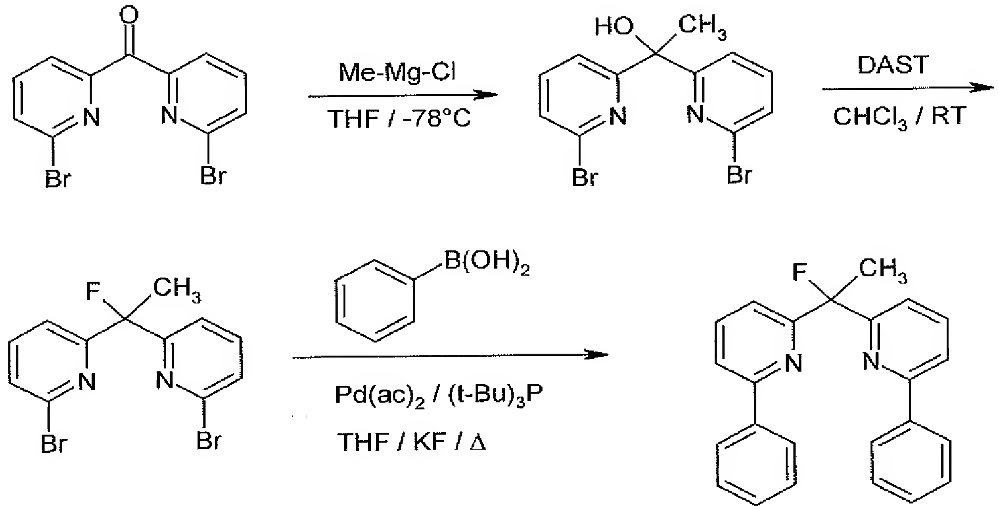
The above compounds (31) to (60) are those already described in detail in structure 2

structure 2

and follow the same concept (V=Z).
These compounds are valuable intermediates on the route to the compounds of structure 1 according to the invention.

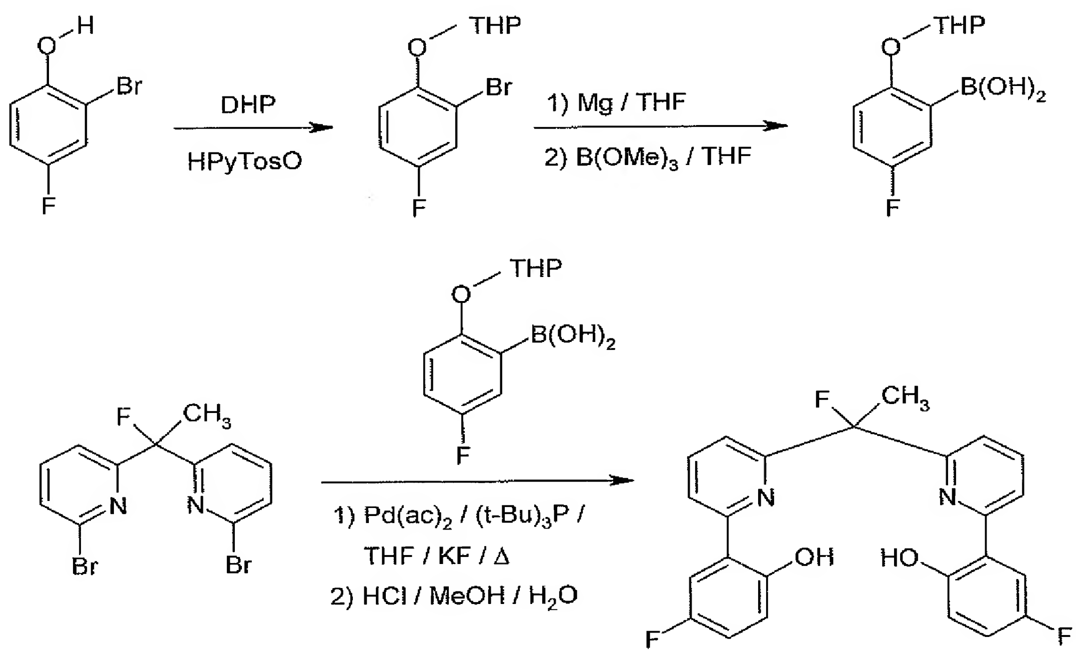
Compounds (31) to (60) according to the invention can be prepared by common organic reaction steps, which is confirmed below with reference to a sufficient number of examples. Thus, compounds (31) can be obtained starting from di(6-bromo-2-pyridyl) ketone (see WO 98/22148) by reaction with aliphatic or aromatic lithium or Grignard reagents, giving a dipyridylmethanol. This can then be fluorinated, chlorinated or brominated, for example by reaction with halogenating agents, such as diethylaminosulfur trifluoride (DAST), thionyl chloride or phosphorus tribromide respectively. Alkylation of the hydroxyl group with formation of an ether can likewise easily be carried out. Final Suzuki coupling with arylboronic acids then gives the compounds (31). This reaction sequence is shown in Scheme 5 with reference to a specific example – methylation, fluorination, coupling with phenylboronic acid – and gives compound (31) where c = 0.

Scheme 5:



An analogous reaction sequence using tetrahydropyranyl-protected phenolboronic acids, which can be prepared from the corresponding bromophenols by protection using dihydropyran, subsequent Grignard reaction and reaction with a boric acid ester, gives, after protecting group removal, compounds of type (31) where c = 1 (Scheme 6).

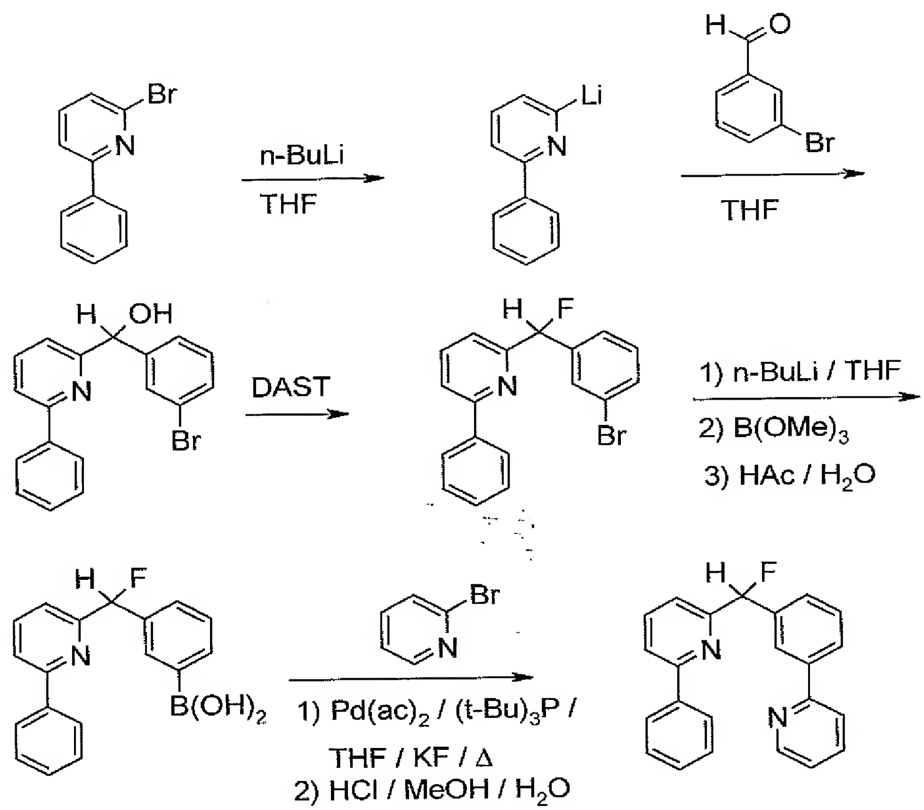
Scheme 6:



Compounds (32) to (38) can also be prepared in an analogous manner through the use of the corresponding 5- and 6-membered heterocyclic compounds.

Compounds of type (39) and (40) can be prepared, for example, in accordance with the reaction sequence shown in Scheme 7 with reference to a specific example. It is of course also possible to obtain a multiplicity of further compounds here by variation of the starting materials (aryl halides or boronic acids).

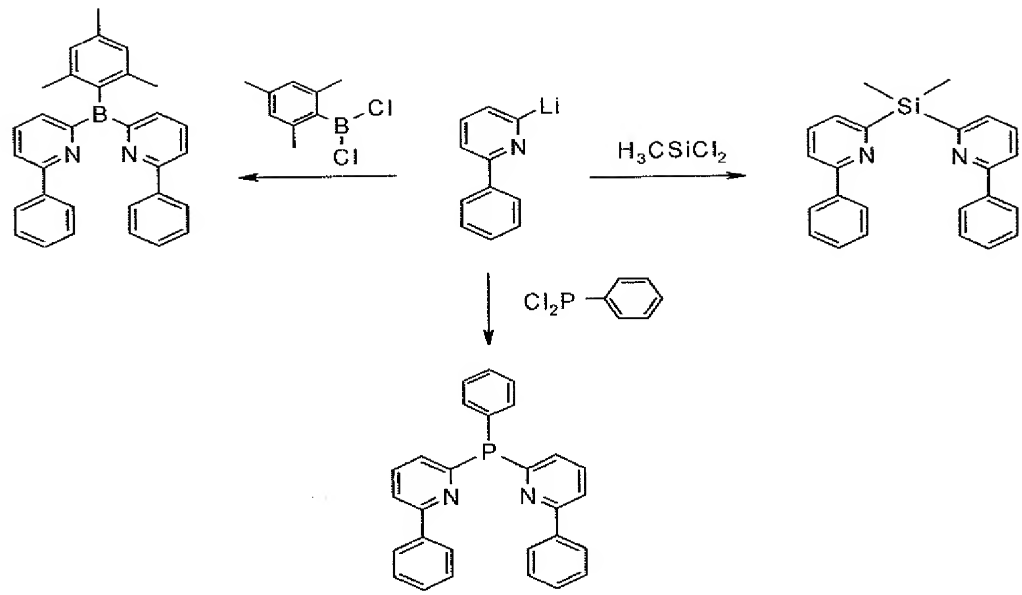
Scheme 7:



Finally, it should be noted that compounds (41) to (60) are also accessible in an entirely analogous manner through the use of analogous reaction sequences.

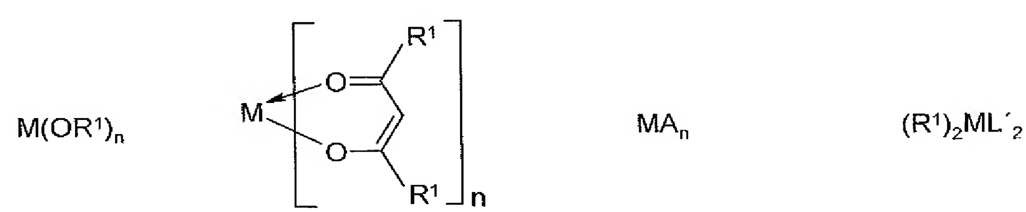
Starting from 2-lithio-6-phenylpyridine and analogues thereof, it is possible to prepare ligands according to the invention which carry heteroatoms in bridge V or Z, it being possible to use electrophiles containing the heteroatom which are suitable as further synthones. Suitable electrophiles are, inter alia, dichloroarylboranes, dichloroalkyl- or -arylsilanes or dichloroaryl- or -alkylphosphines, as is shown in Scheme 8.

Scheme 8:



Compounds (1) to (30) according to the invention can in principle be prepared by various processes, but the novel processes described below have proven particularly suitable.

The present invention therefore furthermore relates to processes for the preparation of compounds (1) to (30) by reaction of the tetradentate chelating ligands as for compounds (31) to (60) with metal alkoxides of the formula (61), with metal ketoketonates of the formula (62), metal halides, carboxylates, nitrates and sulfates of the formula (63) and alkyl- or arylmetal compounds of the formula (64),

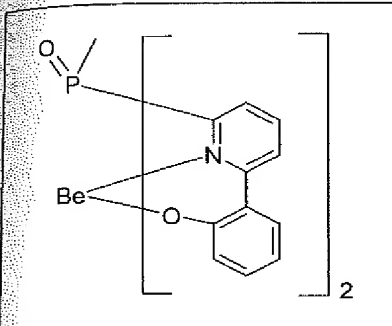
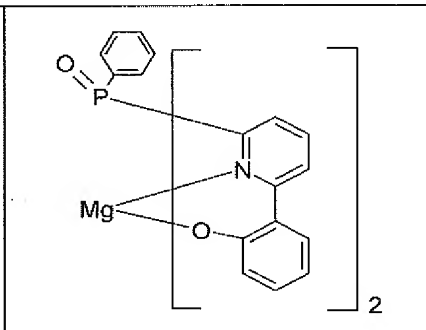
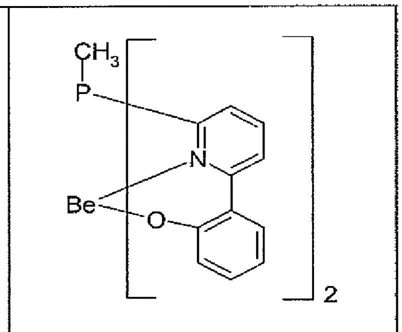
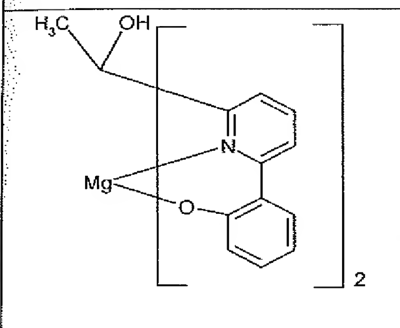
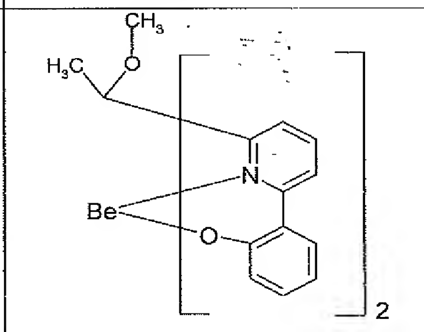
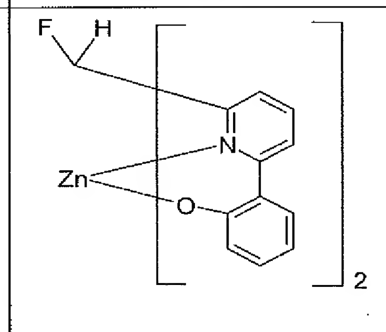
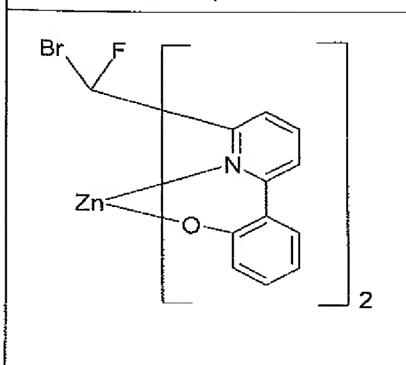
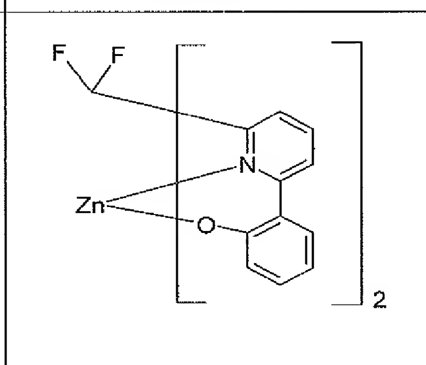
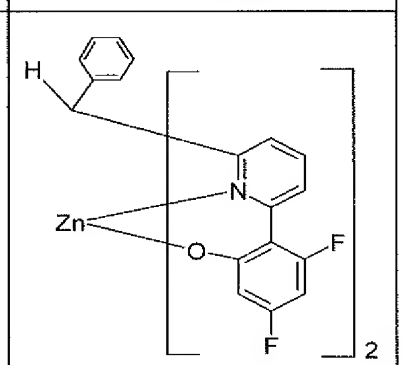


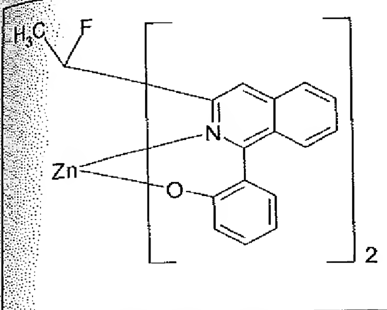
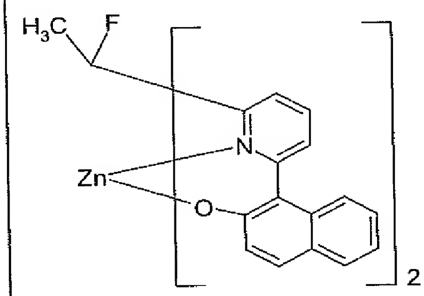
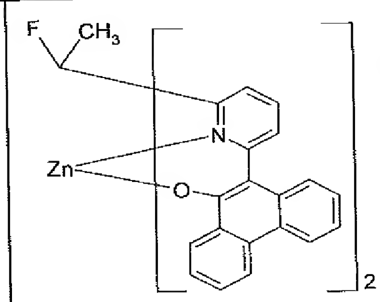
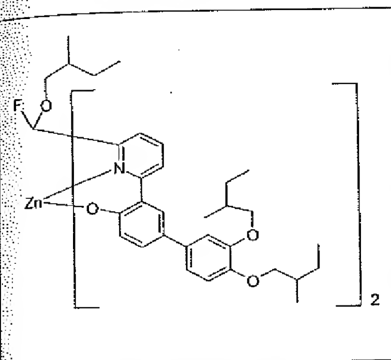
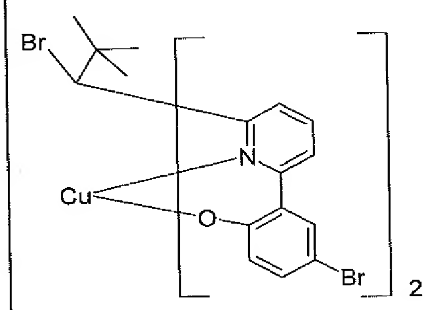
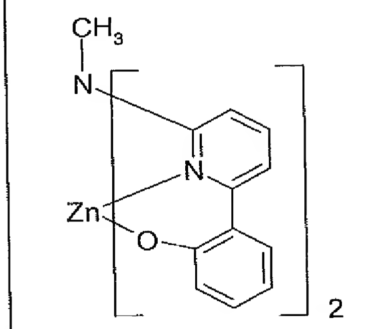
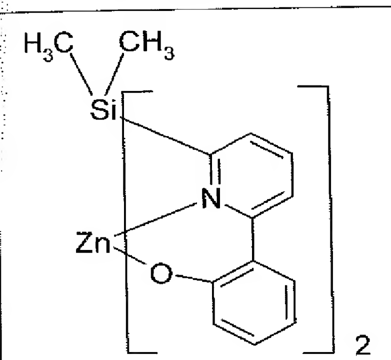
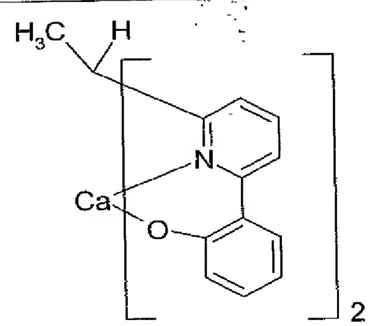
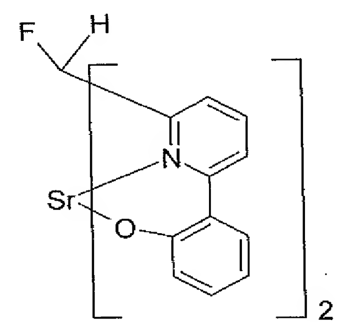
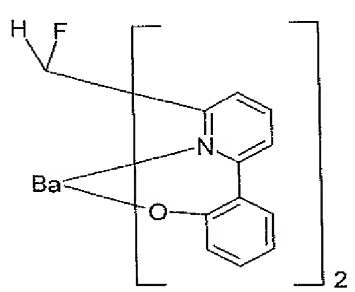
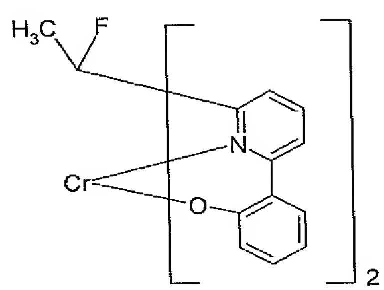
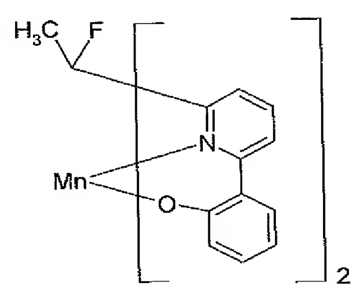
compounds (61) **compounds (62)** **compounds (63)** **compounds (64)**

where the symbols M and R^1 have the meaning indicated under Scheme 1, and A = F, Cl, Br, I , formate, acetate, propionate, benzoate, nitrate, sulfate, and L' is a monodentate ligand from the group of the ethers, such as, for example, THF, the amines, such as, for example, trimethylamine or pyridine, the phosphines, such as, for example, triphenylphosphine, or the sulfoxides, such as, for example, DMSO,

and n = 1, 2, 3. If desired, Lewis acids, such as, for example, aluminium chloride or antimony pentafluoride or -chloride, or Brönsted bases, such as, for example, amines, or alkylating agents, such as, for example, organolithium or Grignard compounds, can be added as auxiliary agents.

The synthetic methods explained here can be used to prepare, inter alia, the examples of compounds (1) to (30) depicted below.

		
Example 1	Example 2	Example 3
		
Example 4	Example 5	Example 6
		
Example 7	Example 8	Example 9

		
Example 10	Example 11	Example 12
		
Example 13	Example 14	Example 15
		
Example 16	Example 17	Example 18
		
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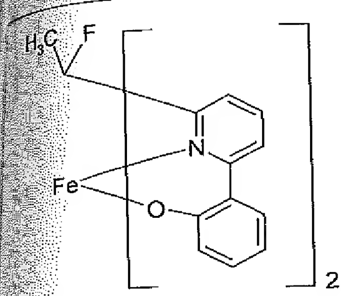	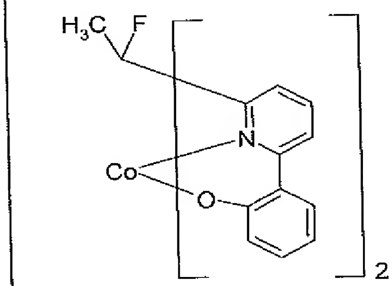	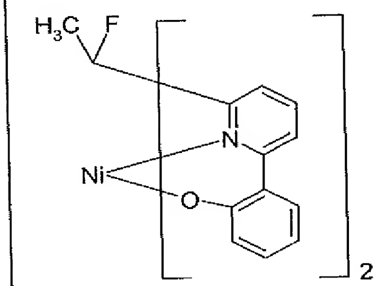
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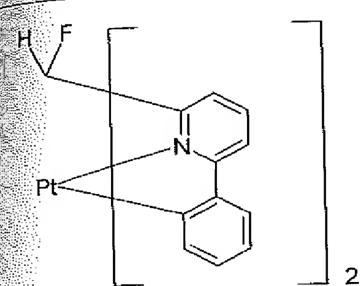	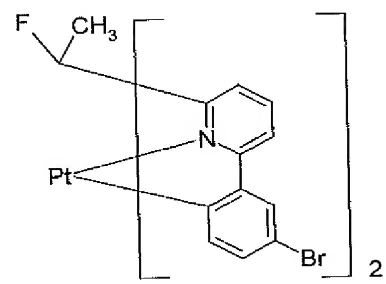	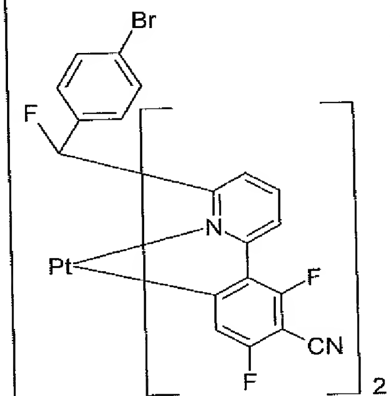
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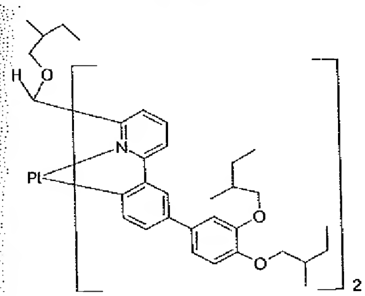	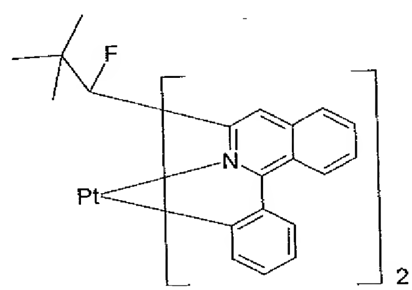	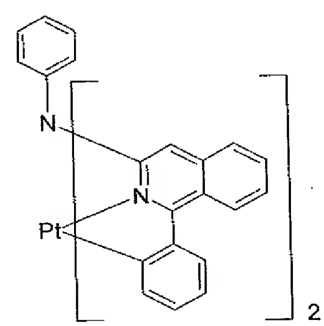
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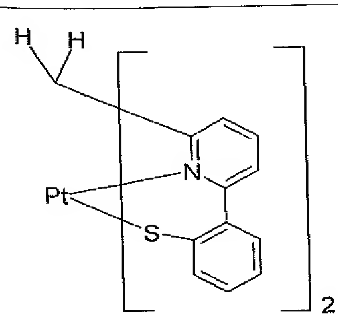	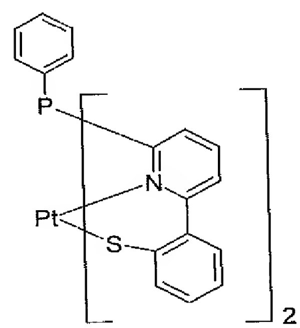	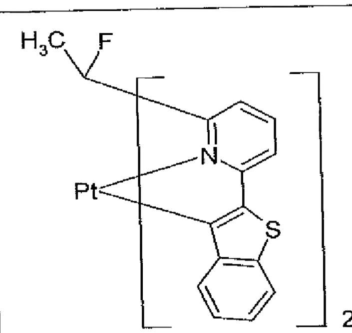
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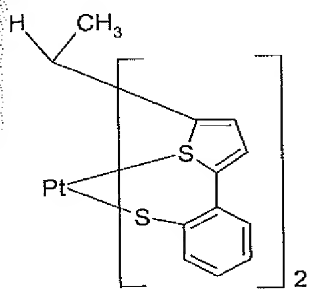	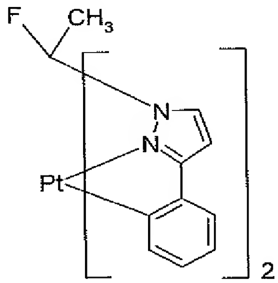	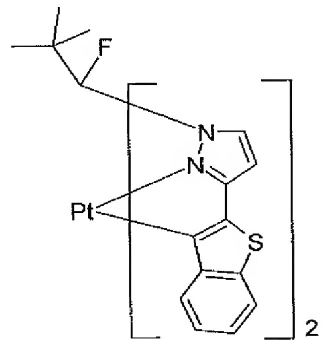
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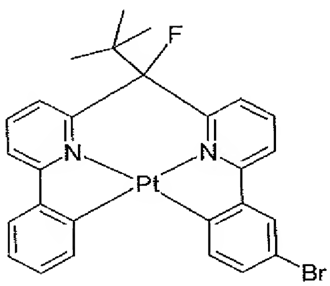	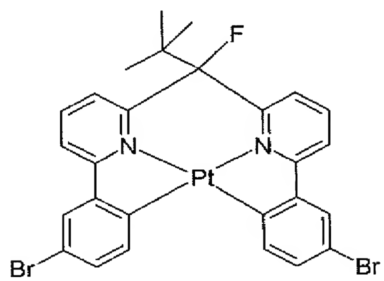	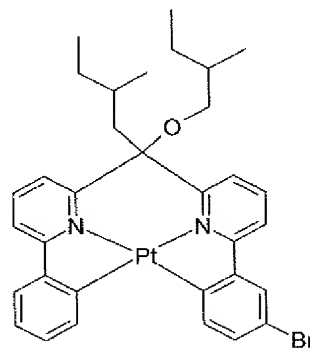
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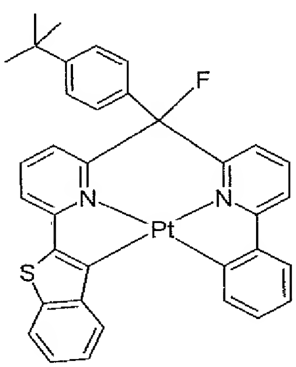	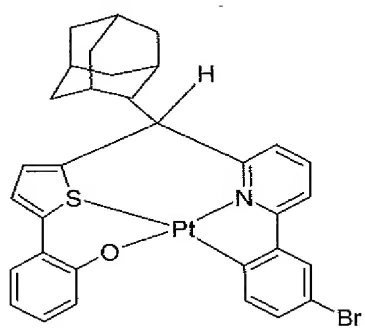	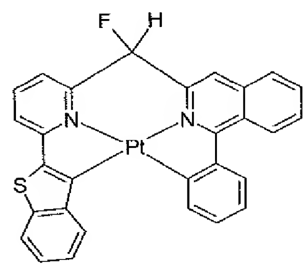
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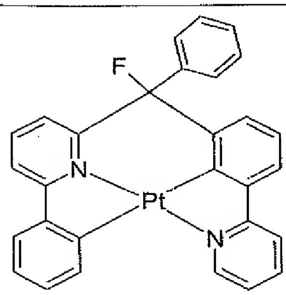	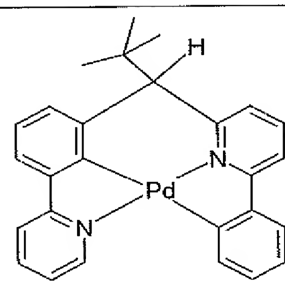	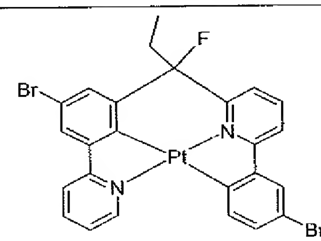
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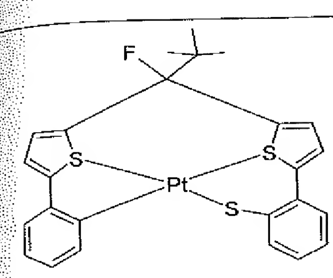	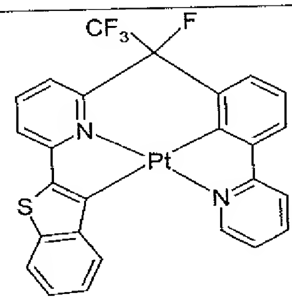	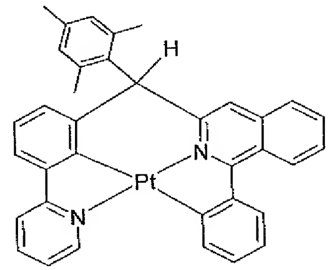
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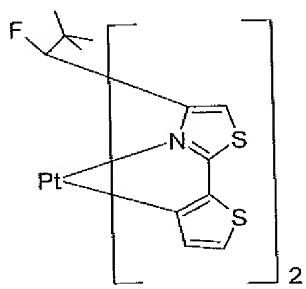	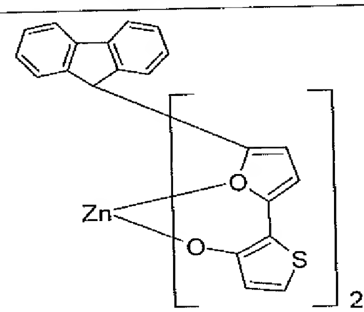	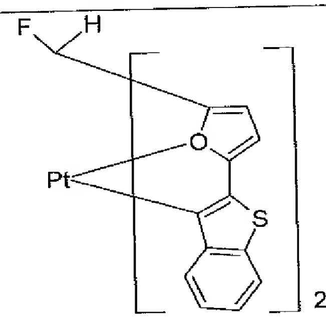
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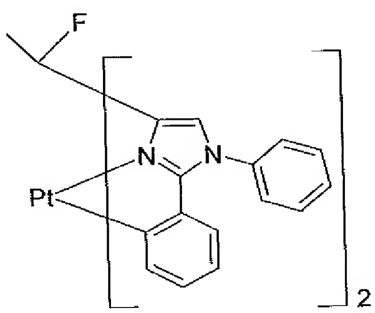	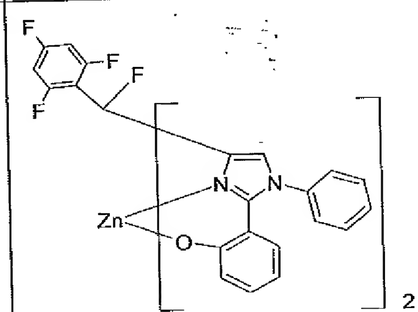	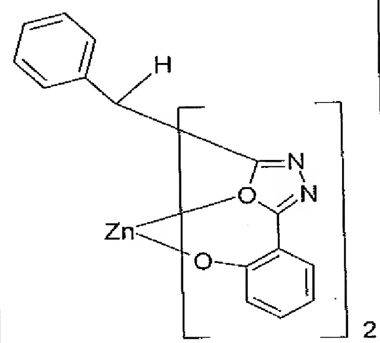
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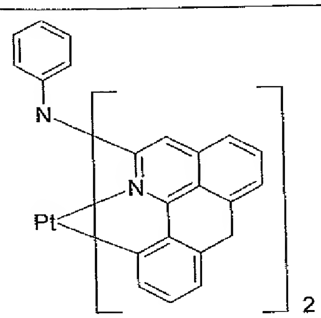	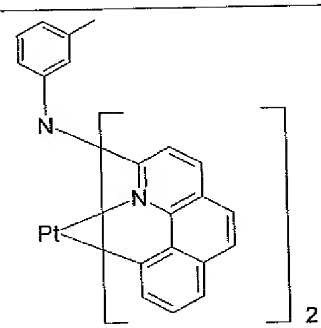	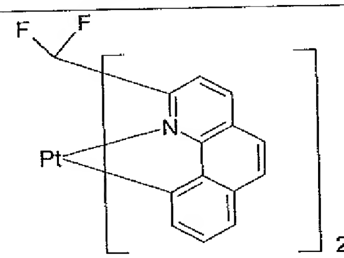
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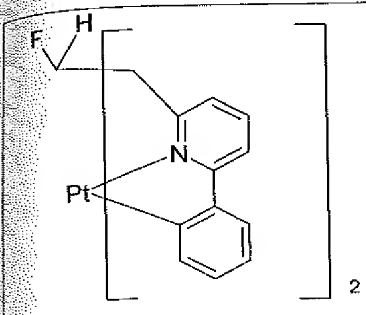
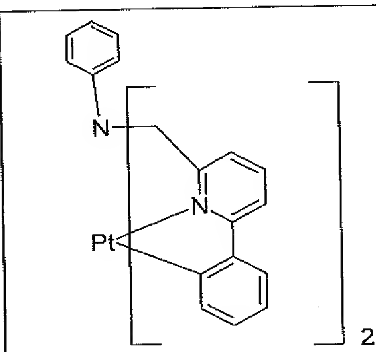
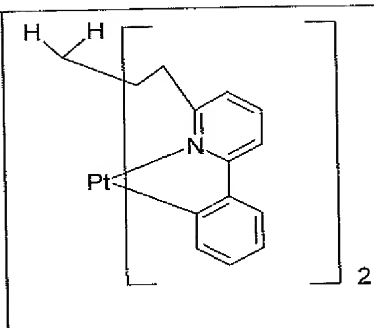
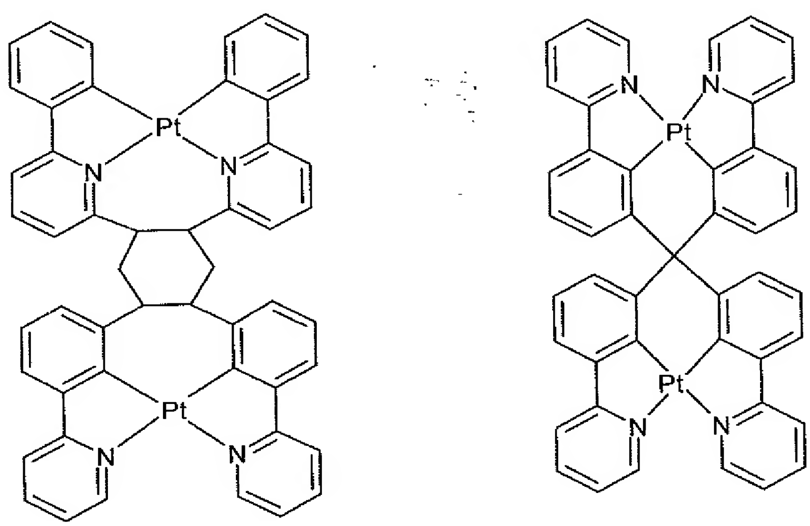
		
Example 58	Example 59	Example 60

In general, structures which contain the above structural elements as substructures, for example the compounds according to Scheme 9, are also regarded as in accordance with the invention.

Scheme 9:



The compounds according to the invention described above - for example compounds according to Examples 7, 14, 26, 27, 37, 38, 39, 41, 45 – can also be used as comonomers for the production of corresponding conjugated, partially conjugated or non-conjugated polymers or dendrimers - for example compounds according to Examples 14 and 26. The corresponding copolymerisation is preferably carried out here via the halogen functionality.
Thus, they can be copolymerised, inter alia, into soluble polyfluorenes (for example in accordance with EP-A-842208 or WO 00/22026), polyspirobifluorenes (for example in accordance with EP-A-707020 or EP-A-894107), poly-para-phenylenes (for example in accordance with WO 92/18552), polydihydrophenanthrenes (for example

in accordance with DE 10337346.2), polycarbazoles (for example in accordance with DE10304819.7 or DE10328627.6), polythiophenes (for example in accordance with EP-A-1028136), polyvinylcarbazoles or also polyketones.

The invention thus furthermore relates to conjugated or partially conjugated polymers or dendrimers containing one or more compounds of the formula (1) to (30), where the R defined above represents a bond to the conjugated, partially conjugated or non-conjugated polymer or dendrimer.

The conjugated or partially conjugated polymers based on polyfluorenes are preferably the polyfluorenes dosclosed in EP-A-842208 and WO 00/22026.

The conjugated or partially conjugated polymers based on polyspirobifluorenes are preferably the polyspirobifluorenes dosclosed in EP-A-707020 and EP-A-894107.

The conjugated or partially conjugated polymers based on poly-para-phenylenes are preferably the poly-para-phenylenes dosclosed in WO 92/18552.

The conjugated or partially conjugated polymers based on polydihydrophenanthrenes are preferably the polydihydrophenanthrenes dosclosed in DE10337345.2.

The conjugated or partially conjugated polymers based on polycarbazoles are preferably the polycarbazoles dosclosed in DE10304819.7 and DE10328627.6.

The conjugated or partially conjugated polymers based on polythiophenes are preferably the polythiophenes dosclosed in EP-A-1028136.

Conjugated, partially conjugated or non-conjugated copolymers comprising the above-mentioned polymer units or polymer building blocks, comprise comprising one or more compounds of the formula (1) to (30), where the R defined above represents a bond to the conjugated, partially conjugated or non-conjugated copolymers, are likewise in accordance with the invention.

The metal complexes according to the invention can furthermore also be functionalised further by the above-mentioned types of reaction, for example, and thus converted into *extended metal complex*. An example which may be mentioned here is functionalisation using arylboronic acids by the SUZUKI method or using amines by the HARTWIG-BUCHWALD method.

compounds (1) to (30) according to the invention described above, the polymers and dendrimers containing compounds of type (1) to (30) as comonomers, and the extended metal complexes are used as active components in electronic components, such as, for example, organic light-emitting diodes (OLEDs), organic integrated circuits (O-ICs), organic field-effect transistors (OFETs), organic thin-film transistors (OTFTs), organic solar cells (O-SCs) or also organic laser diodes (O-lasers).

The invention thus also relates to the use of compounds (1) to (30) according to the invention described above, the polymers and dendrimers containing compounds of type (1) to (30) as comonomers, and the extended metal complexes in electrical devices, such as, for example, organic light-emitting diodes (OLEDs), organic integrated circuits (O-ICs), organic field-effect transistors (OFETs), organic thin-film transistors (OTFTs), organic solar cells (O-SCs) or also organic laser diodes (O-lasers).

The invention furthermore relates to organic light-emitting diodes (OLEDs), organic integrated circuits (O-ICs), organic field-effect transistors (OFETs), organic thin-film transistors (OTFTs), organic solar cells (O-SCs) or organic laser diodes (O-lasers), comprising one or more of compounds (1) to (30) according to the invention, the polymers and dendrimers containing compounds of type (1) to (30) as comonomers, and the extended metal complexes.

The present invention is explained in greater detail by the following examples, without wishing to be restricted thereto. The person skilled in the art will be able to prepare further complexes according to the invention or use the process according to the invention from the descriptions without inventive step.

The OLEDs comprising one or more of the compounds according to the invention can be prepared by processes familiar to the person skilled in the art, as described, for example, in DE 10261545.4 and DE 10317556.3.

Examples:

The following syntheses were, unless indicated otherwise, carried out under a protective-gas atmosphere in dried solvents. The starting materials were purchased from ALDRICH or ABCR [methylmagnesium chloride 3M in THF, diethylaminosulfur trifluoride (DAST), benzeneboronic acid, potassium fluoride (spray-dried), tri-*tert*-butylphosphine, palladium(II) acetate, potassium tetrachloroplatinate]. Di(6-bromo-2-

pyridyl) ketone was prepared as described in WO 98/22148. *cis*-Dimethyl-di(η^1-S-dimethylsulfoxidyl)platinum(II) was prepared as described by C. Eaborn et al., *J. Chem. Soc., Dalton Trans.*, **1981**, 933-938.

Ligand synthesis

Example 1: 1,1-Bis(6-phenyl-2-pyridyl)-1-fluoroethane

a) 1,1-Bis(6-bromo-2-pyridyl)ethan-1-ol

113 ml (340 mmol) of a 3M methylmagnesium chloride solution in THF were added dropwise with vigorous stirring to a suspension, cooled to -78°C, of 102.6 g (300 mmol) of di(6-bromo-2-pyridyl) ketone in 1000 ml of THF at such a rate that a temperature of -60°C was not exceeded. When the addition was complete, the mixture was stirred for a further 30 min., then 50 ml of ethanol were added dropwise, the mixture was warmed to 0°C, and 60 ml of semi-saturated ammonium chloride solution were added. The reaction mixture was filtered, the salts were washed twice with 100 ml of THF each time, and the filtrate was evaporated to dryness in a rotary evaporator. The oily residue was taken up in 1000 ml of dichloromethane, and the organic phase was washed three times with 300 ml of water and then dried over magnesium sulfate. Stripping off of the dichloromethane left 106.0 g (296 mmol), corresponding to a yield of 98.6%, of the crude product having a purity of about 95% according to ^{1}H-NMR as a yellow-brown oil, which was reacted further without purification.

^{1}H-NMR ($CDCl_3$): δ [ppm] = 7.77 (d, $^3J_{HH}$ = 7.8 Hz, 2H), 7.53 (dd, $^3J_{HH}$ = 7.8 Hz, $^3J_{HH}$ = 7.8 Hz , 2H), 7.34 (d, $^3J_{HH}$ = 7.8 Hz, 2H), 5.78 (br. s, 1H, OH), 1.92 (s, 3H, CH_3).

b) 1,1-Bis(6-bromo-2-pyridyl)-1-fluoroethane

117.3 ml (888 mmol) of DAST were added dropwise over the course of 30 min. to a solution, cooled to 10°C, of 105.9 g (296 mmol) of 1,1-bis(6-bromo-2-pyridyl)ethan-1-ol in 1500 ml of chloroform at such a rate that the temperature did not exceed 20°C. The reaction mixture was stirred at 20°C for 1 h and then hydrolysed dropwise with 500 ml of ice-water (care: highly exothermic reaction) with ice cooling and subsequently with 1000 ml of aqueous 3M NaOH. The organic phase was separated off, the aqueous phase was extracted twice with 100 ml of chloroform, and the combined org. phases were washed once with 500 ml of water and dried over calcium chloride. After the desiccant had been filtered off, the brown org. phase was concentrated to 200 ml and filtered through a silica-gel column. The yellow solution obtained in this way was evaporated to dryness, and the yellow, viscous oil remaining was recrystallised from 200 ml of *n*-heptane, giving 78.6 g (218 mmol) of the pro-

duct, corresponding to a yield of 73.7%, in the form of colourless crystal needles – purity according to ^{1}H-NMR > 99.0%.
^{1}H-NMR ($CDCl_3$): δ [ppm] = 7.56 (dd, $^{3}J_{HH}$ = 7.8 Hz, $^{3}J_{HH}$ = 7.8 Hz , 2H), 7.50 (d, $^{3}J_{HH}$ = 7.8 Hz, 2H), 7.34 (d, $^{3}J_{HH}$ = 7.8 Hz, 2H), 2.15 (d, $^{3}J_{HF}$ = 23.4 Hz, 3H, CH_3).

c) 1,1-Bis(6-phenyl-2-pyridyl)-1-fluoroethane
600 µl (2.6 mmol) of tri-tert-butylphosphine and 449 mg (2.0 mmol) of palladium(II) acetate were added to a degassed suspension of 18.0 g (50 mmol) of 1,1-bis(6-bromo-2-pyridyl)-1-fluoroethane, 24.4 g (200 mmol) of benzeneboronic acid and 19.2 g (330 mmol) of potassium fluoride in 350 ml of THF, and the mixture was heated under reflux for 3 h with stirring. After cooling, the THF was removed under reduced pressure, and the residue was taken up in 500 ml of dichloromethane and washed three times with 300 ml of water. After drying over magnesium sulfate, filtration through silica gel and stripping-off of the solvent, the yellow oil remaining was recrystallised three times from ethanol, giving 15.7 g (44 mmol) of the product, corresponding to a yield of 88.6%, in the form of colourless crystal needles - purity according to ^{1}H-NMR > 99%.
^{1}H-NMR ($CDCl_3$): δ [ppm] = 8.04 (d, $^{3}J_{HH}$ = 7.7 Hz, 4H), 7.72 (dd, $^{3}J_{HH}$ = 7.8 Hz, $^{3}J_{HH}$ = 7.8 Hz , 2H), 7.63 (d, $^{3}J_{HH}$ = 7.8 Hz, 2H), 7.50 (d, $^{3}J_{HH}$ = 7.8 Hz, 2H), 7.44 - 7.35 (m, 6H), 2.35 (d, $^{3}J_{HF}$ = 23.4 Hz, 3H, CH_3).

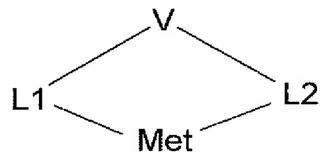
Complex synthesis

Example 1: [1,1-Bis(6-phenyl-2-pyridinato-N,C^{2})-1-fluoroethane]platinum(II)

A solution of 1.063 g (3.0 mmol) of 1,1-bis(6-phenyl-2-pyridyl)-1-fluoroethane and 1.144 g (3.0 mmol) of *cis*-dimethyl-di(η^{1}-S-dimethylsulfoxidyl)platinum(II) in 15 ml of toluene was stirred at 90°C for 3 h. After cooling to room temperature, 30 ml of diethyl ether were added to the yellow suspension, and the yellow, microcrystalline product was filtered off with suction and washed three times with 10 ml of diethyl ether each time. Drying under reduced pressure gave 1.544 g (2.8 mmol), corresponding to a yield of 94.0%, having a purity > 99.5% (HPLC).
MS (FAB): m/e = 347 (M+).

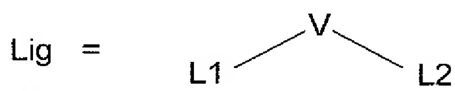
Patent Claims:

1. Compounds of structure 1 characterised in



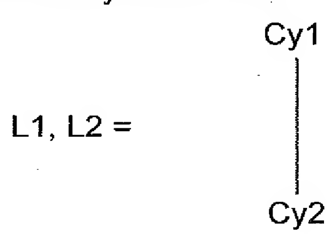
structure 1

that they contain a metal Met, coordinated to a tetradentate chelating ligand Lig of structure 2



structure 2

where V is a bridging unit, characterised in that it contains 1 to 40 atoms heavier than hydrogen and connects the two ligand moieties L1 and L2, which may be identical or different on each occurrence, covalently to one another, and where the two ligand moieties L1 and L2 satisfy structure 3



structure 3

where Cy1 and Cy2, identically or differently on each occurrence, correspond to a substituted or unsubstituted, saturated, unsaturated or aromatic homo- or heterocycle, which is in each case bonded ionically, covalently or coordinatively to the metal via a ring atom or via an atom bonded exocyclically to the homo- or heterocycle.

2. Compounds according to Claim 1, characterised in that they are electrically neutral.

3. Compounds according to Claim 1 and / or 2, characterised in that L1 = L2.

4. Compounds according to one or more of Claims 1 to 3, characterised in that the linking unit V contains one, two or three bridging atoms or is a 3- to 6-membered homo- or heterocycle.

5. Compounds according to one or more of Claims 1 to 4, characterised in that the linking unit V contains a linking atom selected from the 3rd, 4th, 5th or 6th main group

6. Compounds according to one or more of Claims 1 to 5, characterised in that the linking unit

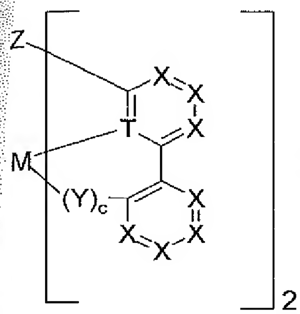
V stands for BR^1, $-(CR_2)R^1B(CR_2)-$, $-(CR_2CR_2)R^1B(CR_2CR_2)-$, C=O, $C=NR^1$, C=S, CR_2, CR(OH), $CR(OR^1)$, $C(NR^1)_2$, $-(CR_2)R_2C(CR_2)-$, $-(CR_2CR_2)R_2C(CR_2CR_2)-$, $-(SiR_2)R_2C(SiR_2)-$, $-(SiR_2CR_2)R_2C(SiR_2CR_2)-$, $-(CR_2SiR_2)R_2C(CR_2SiR_2)-$, $-(SiR_2SiR_2)R_2C(SiR_2SiR_2)-$, cis-RC=CR, 1,2-$C_6H_4$, 1,3-$C_6H_4$, SiR_2, $Si(OH)_2$, $Si(OR^1)_2$, $-(CR_2)R_2Si(CR_2)-$, $-(CR_2CR_2)R_2Si(CR_2CR_2)-$, $-(SiR_2)R_2Si(SiR_2)-$, $-(SiR_2CR_2)R_2Si(SiR_2CR_2)-$, $-(CR_2SiR_2)R_2Si(CR_2SiR_2)-$, $-(SiR_2SiR_2)R_2Si(SiR_2SiR_2)-$, R^1N, $-(CR_2)R^1N(CR_2)-$, $-(CR_2CR_2)R^1N(CR_2CR_2)-$, FP, FPO, R^1P, R^1As, R^1Sb, R^1Bi, R^1PO, R^1AsO, R^1SbO, R^1BiO, R^1PSe, R^1AsSe, R^1SbSe, R^1BiSe, R^1PTe, R^1AsTe, R^1SbTe, R^1BiTe, O, S, Se, $-(CR_2)O(CR_2)-$, $-(CR_2)S(CR_2)-$, $-(CR_2)(O)S(CR_2)-$, $-(CR_2)(O)_2S(CR_2)-$;

and

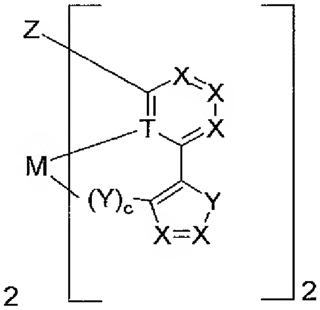
R is, identically or differently on each occurrence, H, F, Cl, Br, I, NO_2, CN, a straight-chain, branched or cyclic alkyl or alkoxy group having 1 to 20 C atoms, where one or more non-adjacent CH_2 groups may be replaced by -O-, -S-, $-NR^1-$ or $-CONR^2-$ and where one or more H atoms may be replaced by F, or an aryl or heteroaryl group having 1 to 14 C atoms, which may be substituted by one or more non-aromatic radicals R, where a plurality of substituents R, both on the same ring and also on the two different rings, may in turn form a further mono- or polycyclic, aliphatic or aromatic ring system; and

R^1 and R^2, identically or differently on each occurrence, denote H or an aliphatic or aromatic hydrocarbon radical having 1 to 20 C atoms.

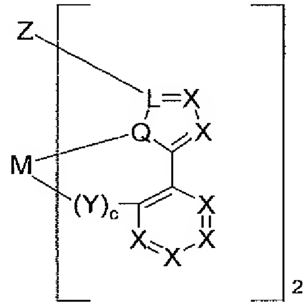
7. Metal complexes according to one or more of Claims 1 to 6, selected from compounds (1) to (8),



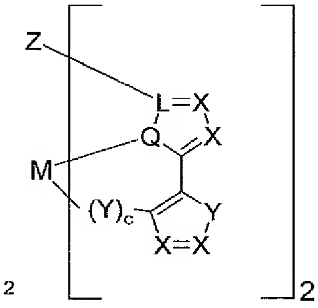
compounds (1)



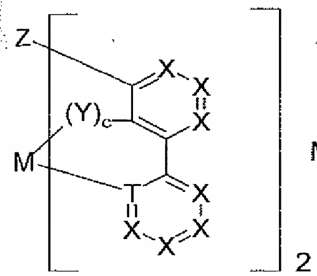
compounds (2)



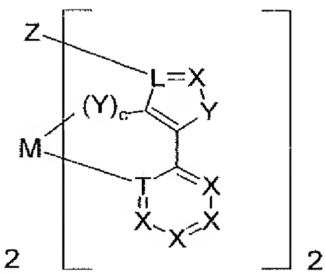
compounds (3)



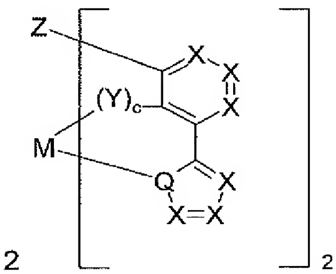
compounds (4)



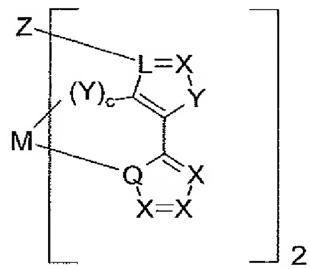
compounds (5)



compounds (6)



compounds (7)



compounds (8)

where the symbols and indices have the following meaning:

M is Be, Mg, Ca, Sr, Ba, Cr, Mo, W, Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag, Au, Zn, Cd or Hg;

L is, identically or differently on each occurrence, C, N or P;

Q is, identically or differently on each occurrence, N, O, S, Se or Te;

T is, identically or differently on each occurrence, N or P;

X is, identically or differently on each occurrence, CR, N or P;

Y is, identically or differently on each occurrence, NR^1, O, S, Se, Te, SO, SeO, TeO, SO_2, SeO_2 or TeO_2;

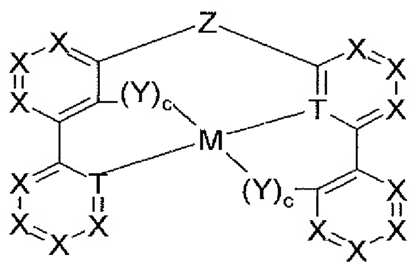
Z BR^1, $-(CR_2)R^1B(CR_2)-$, $-(CR_2CR_2)R^1B(CR_2CR_2)-$, C=O, $C=NR^1$, C=S, CR_2, CR(OH), $CR(OR^1)$, $C(NR^1)_2$, $-(CR_2)R_2C(CR_2)-$, $-(CR_2CR_2)R_2C(CR_2CR_2)-$, $-(SiR_2)R_2C(SiR_2)-$, $-(SiR_2CR_2)R_2C(SiR_2CR_2)-$, $-(CR_2SiR_2)R_2C(CR_2SiR_2)-$, $-(SiR_2SiR_2)R_2C(SiR_2SiR_2)-$, cis-RC=CR, 1,2-$C_6H_4$, 1,3-$C_6H_4$, SiR_2, $Si(OH)_2$, $Si(OR^1)_2$, $-(CR_2)R_2Si(CR_2)-$, $-(CR_2CR_2)R_2Si(CR_2CR_2)-$, $-(SiR_2)R_2Si(SiR_2)-$, $-(SiR_2CR_2)R_2Si(CR_2SiR_2)-$, $-(CR_2SiR_2)R_2Si(SiR_2CR_2)-$, $-(SiR_2SiR_2)R_2Si(SiR_2SiR_2)-$, R^1N, $-(CR_2)R^1N(CR_2)-$, $-(CR_2CR_2)R^1N(CR_2CR_2)-$, FP, FPO, R^1P, R^1As, R^1Sb, R^1Bi, R^1PO, R^1AsO, R^1SbO, R^1BiO, R^1PSe, R^1AsSe, R^1SbSe, R^1BiSe, R^1PTe, R^1AsTe, R^1SbTe, R^1BiTe, O, S, Se, $-(CR_2)O(CR_2)-$, $-(CR_2)S(CR_2)-$, $-(CR_2)(O)S(CR_2)-$, $-(CR_2)(O)_2S(CR_2)-$;

R is, identically or differently on each occurrence, H, F, Cl, Br, I, NO_2, CN, a straight-chain, branched or cyclic alkyl or alkoxy group having 1 to 20 C atoms, where one or more non-adjacent CH_2 groups may be replaced by -O-, -S-, $-NR^1-$ or $-CONR^2-$ and where one or more H atoms may be replaced by F, or an aryl or heteroaryl group having 1 to 14 C atoms, which may be substituted by one or more non-aromatic radicals R, where a plurality of substituents R, both on the same ring and also on the two different rings, may in turn form a further mono- or polycyclic, aliphatic or aromatic ring system;

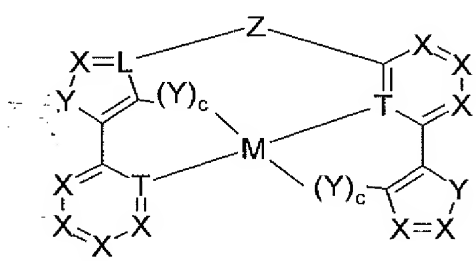
R^1 and R^2, identically or differently on each occurrence, are H or an aliphatic or aromatic hydrocarbon radical having 1 to 20 C atoms.

c is, identically or differently on each occurrence, 0 or 1.

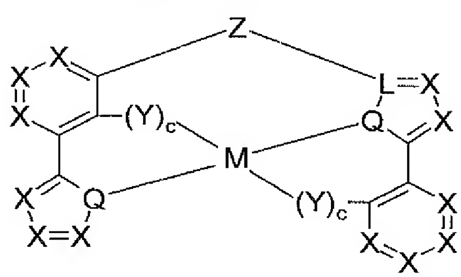
8. Metal complexes according to one or more of Claims 1 to 6, selected from compounds (9) to (12),



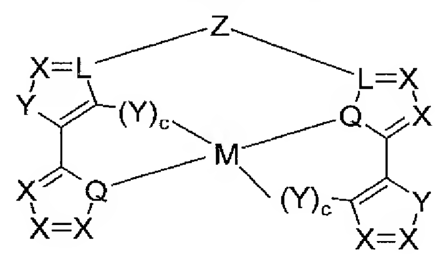
compounds (9)



compounds (10)



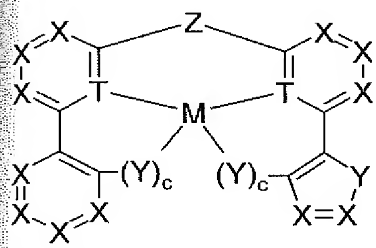
compounds (11)



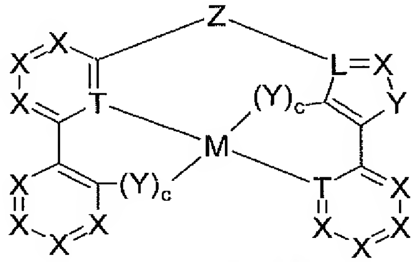
compounds (12)

where the symbols and indices M, L, Q, T, X, Y, Z, R, R^1, R^2 and c have the meanings as in Claim 6.

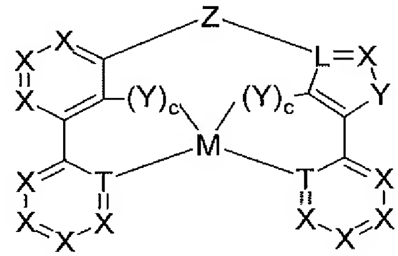
9. Metal complexes according to one or more of Claims 1 to 6, selected from compounds (13) to (30),



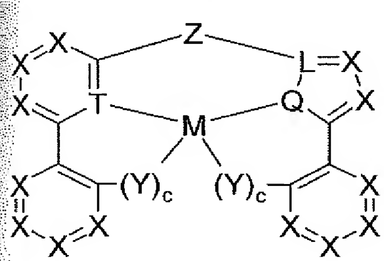
compounds (13)



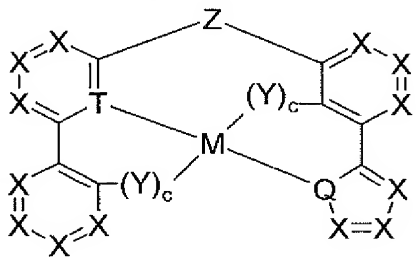
compounds (14)



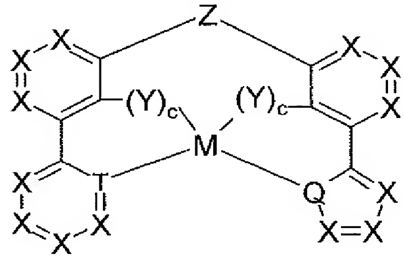
compounds (15)



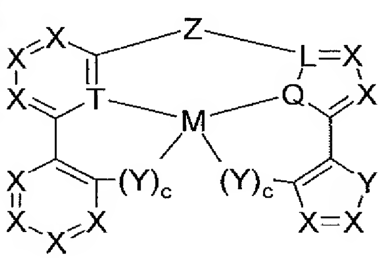
compounds (16)



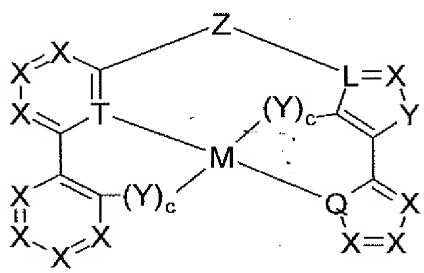
compounds (17)



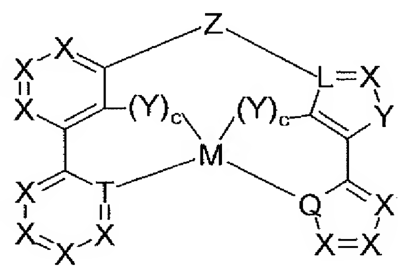
compounds (18)



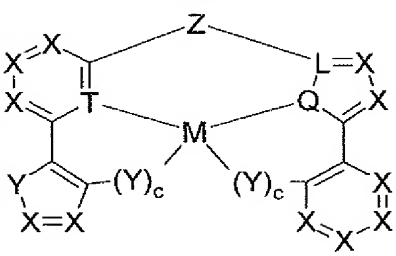
compounds (19)



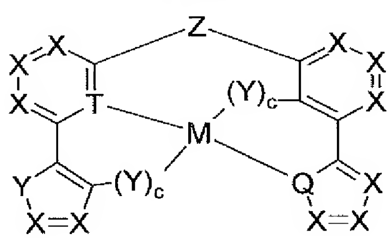
compounds (20)



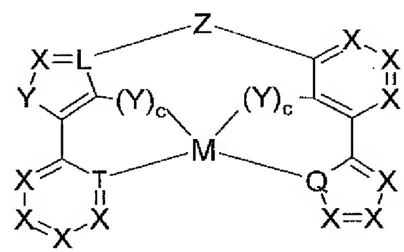
compounds (21)



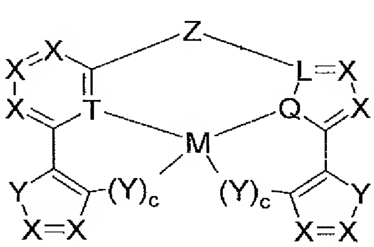
compounds (22)



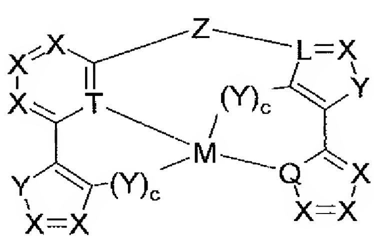
compounds (23)



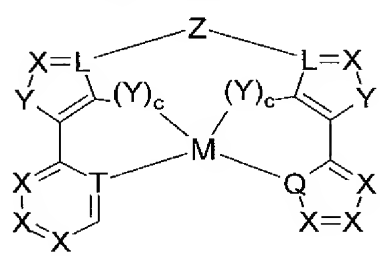
compounds (24)



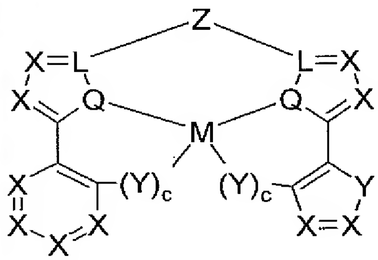
compounds (25)



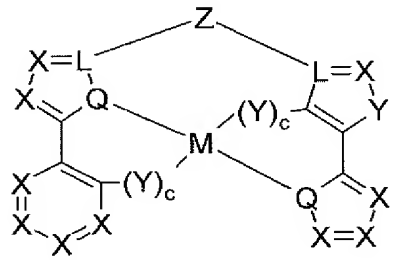
compounds (26)



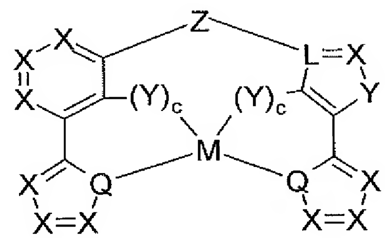
compounds (27)



compounds (28)



compounds (29)

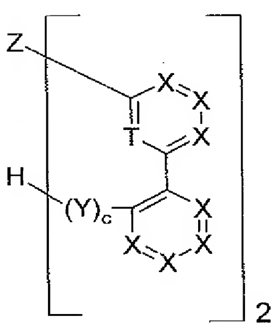


compounds (30)

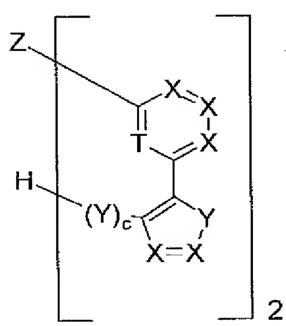
where the symbols and indices M, L, Q, T, X, Y, Z, R, R^1, R^2, c and n have the meanings as in Claim 7.

9. Metal complexes according to one or more of Claims 1 to 8, characterised in that ligand L3, if present, is a bidentate chelating ligand.

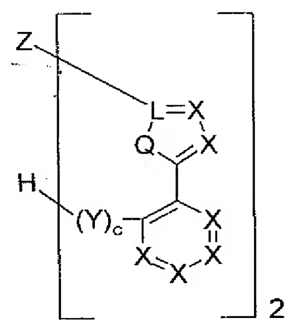
10. Compounds (31) to (60)



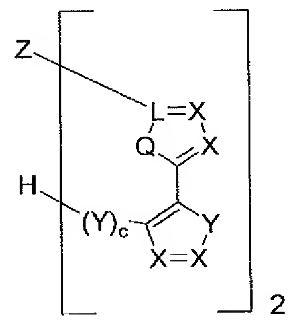
compounds (31)



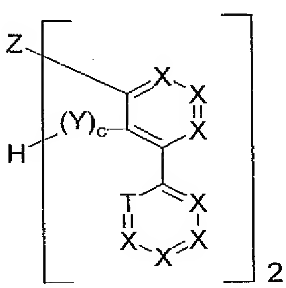
compounds (32)



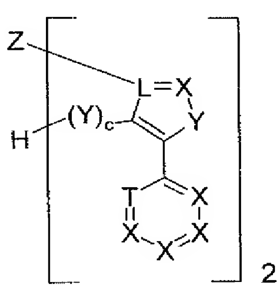
compounds (33)



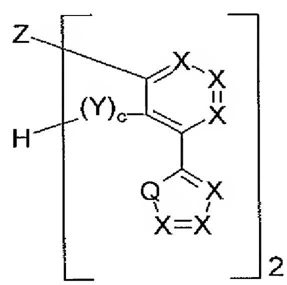
compounds (34)



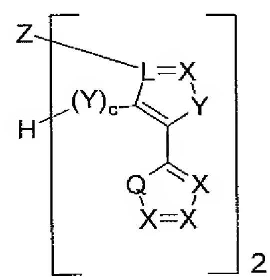
compounds (35)



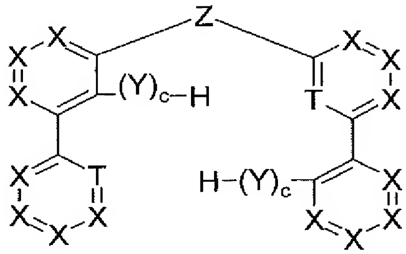
compounds (36)



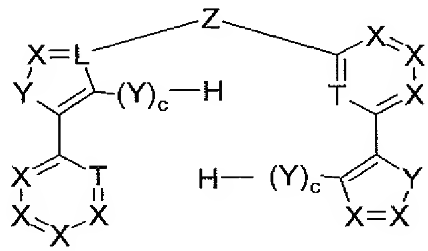
compounds (37)



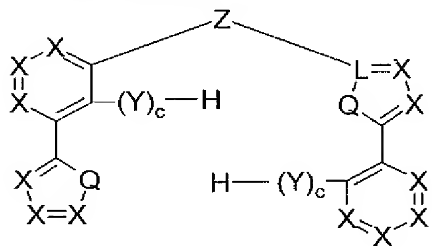
compounds (38)



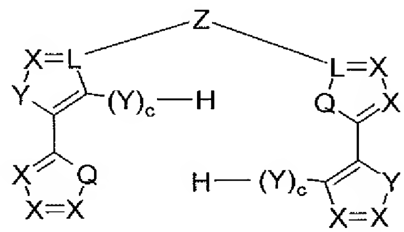
compounds (39)



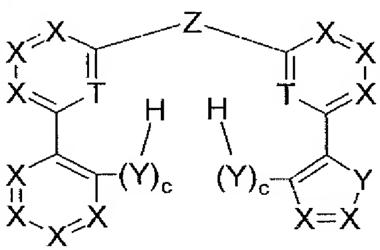
compounds (40)



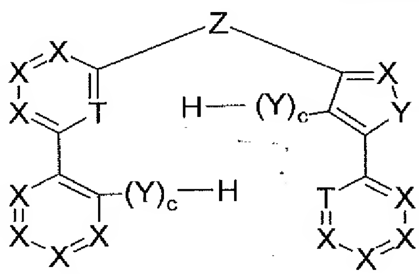
compounds (41)



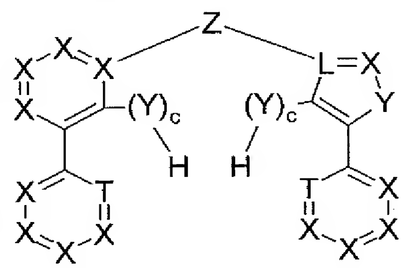
compounds (42)



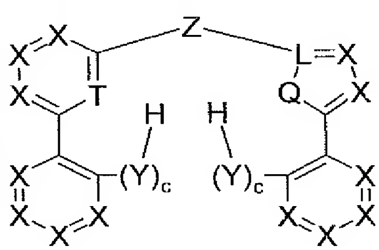
compounds (43)



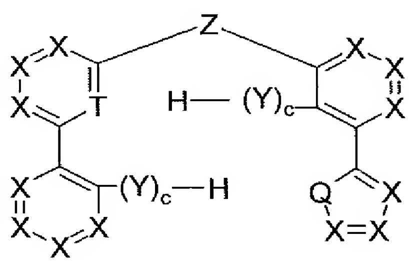
compounds (44)



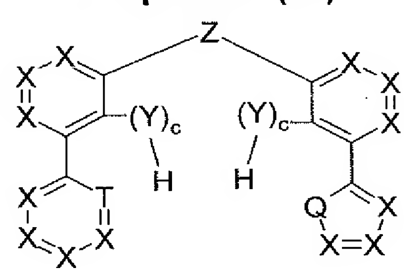
compounds (45)



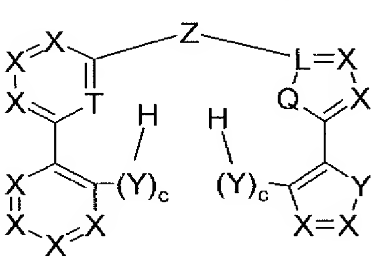
compounds (46)



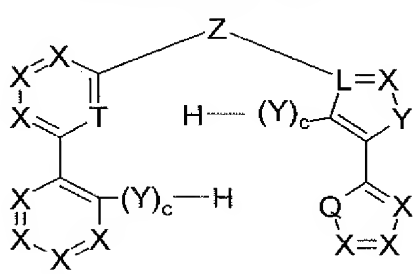
compounds (47)



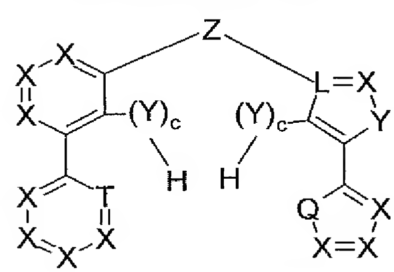
compounds (48)



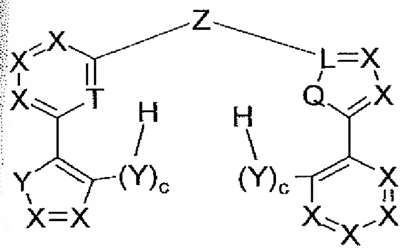
compounds (49)



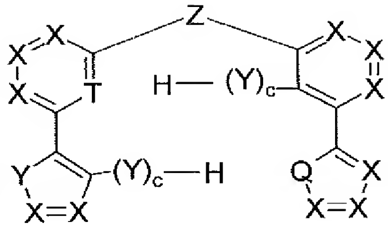
compounds (50)



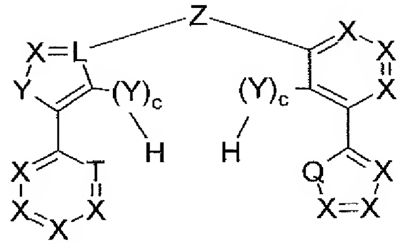
compounds (51)



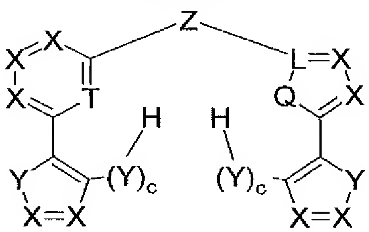
compounds (52)



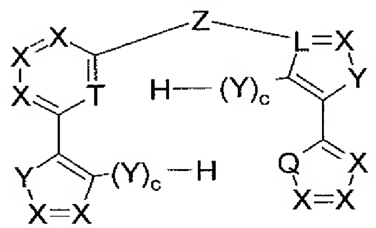
compounds (53)



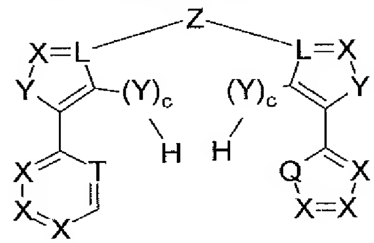
compounds (54)



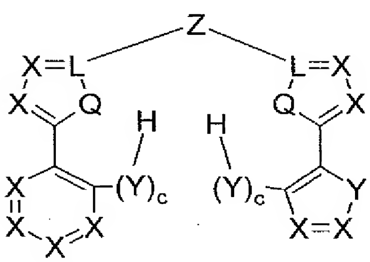
compounds (55)



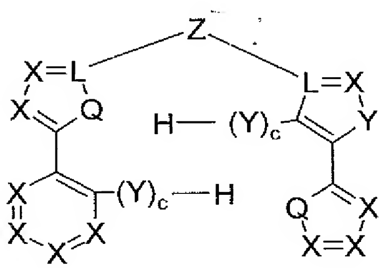
compounds (56)



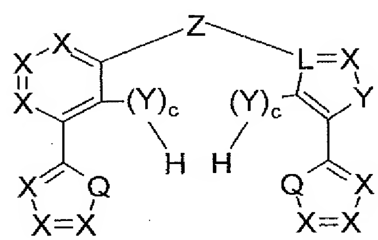
compounds (57)



compounds (58)



compounds (59)



compounds (60)

where the symbols and indices L, Q, T, X, Y, Z, R, R^1, R^2 and c have the meanings as in Claim 6, with the exception of the compounds bis(6-phenyl-2-pyridyl)methane [CAS 362602-93-5], bis(6-phenyl-2-pyridyl) ketone [CAS 217177-35-0], bis(6-(1-hydroxy-3,5-di-tert-butyl)phenyl-2-pyridyl)methanol [CAS 367525-74-4], 2,2′-thio-bis(3-cyano-2,4-diphenyl)pyridine [CAS 160598-76-5], bis(6-(3-phenyl)phenyl-2-pyridyl)methane [CAS 57476-80-9] and isomers [CAS 57476-79-6].

11. Compounds according to one or more of Claims 1 to 9, characterised in that the symbol M = Be, Mg, Pt, Zn.

12 Compounds according to one or more of Claims 1 to 9, characterised in that the symbol c = 0 and M = Pt.

13. Compounds according to one or more of Claims 1 to 10, characterised in that the symbol L = C, N.

14. Compounds according to one or more of Claims 1 to 10, characterised in that the symbol Q = O, S.

15. Compounds according to one or more of Claims 1 to 10, characterised in that the symbol T = N.

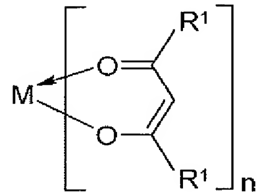
16. Compounds according to one or more of Claims 1 to 10, characterised in that the symbol X = CR, N.

17. Compounds according to one or more of Claims 1 to 10, characterised in that the symbol Z = BR^1, CR_2, CO, SiR^1_2, R^1N, FP, FPO, R^1P, R^1PO, in which R^1, identically or differently on each occurrence, denotes H or an aliphatic or aromatic hydrocarbon radical having 1 to 20 C atoms and R has the meanings as in Claim 18.

18. Compounds according to one or more of Claims 1 to 10, characterised in that the symbol R = H, F, Cl, Br, I, CN, a straight-chain or branched or cyclic alkyl or alkoxy group having 1 to 6 C atoms or an aryl or heteroaryl group having 3 to 10 C atoms, which may be substituted by one or more non-aromatic radicals R, where a plurality of substituents R, both on the same ring and also on the two different rings, may together in turn form a further mono- or polycyclic ring system.

19. Compounds according to one or more of Claims 1 to 10, characterised in that the polycyclic ring system optionally formed by the radical(s) R corresponds to benzene, 1- or 2-naphthalene, 1-, 2- or 9-anthracene, 2-, 3- or 4-pyridine, 2-, 4- or 5-pyrimidine, 2-pyrazine, 3- or 4-pyridazine, triazine, 2-, 3-, 4-, 5-, 6-, 7- or 8-quinoline, 2- or 3-pyrrole, 3-, 4-, 5-pyrazole, 2-, 4-, 5-imidazole, 2-, 3-thiophene, 2-, 3-selenophene, 2- or 3-furan, 2-(1,3,4-oxadiazole), indole or carbazole

20. Process for the preparation of the compounds according to one or more of Claims 1 to 9 by reaction of compounds (31) to (60), according to Claim 10 with metal alkoxides of the formula (61), with metal ketoketonates of the formula (62), metal halides, carboxylates, nitrates and sulfates of the formula (63) or alkyl- or arylmetal compounds of the formula (64)

$M(OR^1)_n$		MA_n	$(R^1)_2ML'_2$
compounds (61)	**compounds (62)**	**compounds (63)**	**compounds (64)**

where the symbols M and R^1 have the meaning given in Claim 7, and the symbol A = F, Cl, Br, I , formate, acetate, propionate, benzoate, nitrate, sulfate, and L' is a monodentate ligand and n = 1, 2, 3.

21. Compounds according to one or more of Claims 1 to 9 and 11 to 19, characterised in that their purity (determined by ^{1}H-NMR and/or HPLC) is greater than 99%.

22. Conjugated, partially conjugated and/or non-conjugated polymers or dendrimers containing one or more compounds of structure (1) or of the formula (1) to (30) according to one or more of Claims 1 to 9 and 11 to 19.

23. Polymers or dendrimers according to Claim 22, characterised in that the R defined in Claim 7 represents a bond to the conjugated, partially conjugated and/or non-conjugated polymer or dendrimer.

24. Polymers according to Claim 22 and / or 23, characterised in that the polymer is selected from the group of the polyfluorenes, polyspirobifluorenes, poly-para-phenylenes, polydihydrophenanthrenes, polycarbazoles, polythiophenes, polyketones, polyvinylcarbazoles or from copolymers which have a plurality of the units mentioned here.

25. Electronic component comprising at least one compound, a polymer, a copolymer or a dendrimer according to one or more of Claims 1 to 9 and 11 to 19 and 22 to 24.

26. Electronic component according to Claim 25, characterised in that it is an organic light-emitting diode (OLED), an organic integrated circuits (O-IC), an organic field-effect transistor (OFET), an organic thin-film transistor (OTFT), an organic solar cell (O-SC) or also an organic laser diode (O-laser).

Abstract C03034

Metal complexes

The present invention describes novel metal complexes. Compounds of this type can be employed as functional materials in a number of applications of different types which can be ascribed to the electronics industry in the broadest sense.

The compounds according to the invention are described by structure 1 and formulae (1) to (60).